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Estimation of thermal conductivity of pure gases by using artificial neural networks

R. Eslamloueyan *, M.H. Khademi

Chemical and Petroleum Engineering Department, School of Engineering, Shiraz University, Zand Avenue, Shiraz, Iran

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ABSTRACT

A feedforward three-layer neural network is proposed to predict conductivity (k) of pure gases at atmospheric pressure and a wide range of temperatures based on their critical temperature (T_c), critical pressure (P_c) and molecular weight (MW). The accuracy of the method is evaluated and tested by its application to experimental conductivities of various gases which some of them are not used in the network training. Furthermore, the performance of the proposed technique is compared with that of conventional recommended models in the literature. The results of this comparison show that the proposed neural network outperforms other alternative methods, with respect to accuracy as well as extrapolation capabilities. Besides, conventional conductivity correlations are usually used for a limited range of temperature and components while the network method is able to cover a wide range of temperatures and substances.

1. Introduction

Thermal conductivity of gases is one of the most important thermal properties, since it is needed in the analysis of heat transfer equipment. Data on thermal conductivity are required for mathematical modeling and computer simulation of heat transfer processes. Over the years, the thermal conductivity has been measured and compiled for many gases. In general, the estimation methods of thermal conductivity can be divided into two broad categories. In one category, thermal conductivity is estimated through using relations based on the theory of gases. The second category consists of correlations relating thermal conductivity to other properties such as critical temperature, critical pressure and molecular weight, which can be easily measured. Table 1 shows most of the methods and correlations currently being used in estimation of thermal conductivity.

Neural networks have been used extensively in various fields of chemical engineering over the last two decades. Turias et al. studied the application of pattern recognition and artificial intelligence techniques in the characterization of a multi-phase realistic disordered composite and in a design of a multiple regression model to estimate effective thermal conductivity [1]. Sablani and Rahman presented an artificial neural network (ANN) model for the prediction of thermal conductivity of food as a function of moisture content, temperature and apparent porosity [2]. The model was able to predict thermal conductivity with a mean relative error of 12.6%. Sablani et al. suggested an artificial neural network model for the prediction of thermal conductivity of bakery products as a function of product moisture content, temperature and apparent density [3]. The model was able to predict thermal conductivity with a mean relative error of 10%. Zhou et al. focused on modeling the electrical conductivity of recombined milk by artificial neural network [4]. They aimed to establish a nonlinear relationship that accounts for the effect of milk constituents (protein, lactose, and fat) and temperature on the electrical conductivity of recombined milk. Jalali-Heravi et al. developed a quantitative structure-activity relationship method using an ANN for predicting the thermal conductivity detector response factor [5].

The objective of this work is to develop a neural network model for prediction of thermal conductivity of pure gases at atmospheric pressure over a wide range of temperatures. The network inputs are the gas temperature, critical temperature, critical pressure and molecular weight. The next section gives a brief overview of the artificial neural network used in this study. Then, the proposed method as well as the data used in its development and validation is presented. Section three contains the results and discussion about the proposed method.

2. Methodology

Considering the inherent ability of artificial neural networks to learn and recognize nonlinear and complex relationships, they can be used to predict conductivity of gases. The proposed method is based on a neuromorphic model. The following steps are those required to develop the neuromorphic models to predict conductivity.

* Corresponding author. Fax: +98 711 6287294.
E-mail address: eslamlo@shirazu.ac.ir (R. Eslamloueyan).

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Nomenclature

b_j	bias of jth neuron
F	activation or transfer function
K	conductivity
MW	molecular weight
N	number of input signals to jth neuron
N	number of data points
O_j	output of jth neuron
P_c	critical pressure
T	temperature
T_c	critical temperature
w_{ji}	synaptic weight corresponding to ith synapse of jth neuron
x_i	ith input signal to jth neuron

Subscripts

exp	experimental
P	predicted

Table 1
The summary of thermal conductivity correlations and methods

Source	Comment
First category	
Pidduck model [6]	The first attempt to treat the case of polyatomic molecules rigorously is the simple model of Bryan, to which Pidduck extended the Chapman–Enskog method for an infinitely dilute gas of spherical molecules to the case of perfectly rough rigid elastic spherical molecules possessing rotational energy that can be converted into translational energy.
The Eucken approximation [7]	He determined the role of internal degree of freedom on conductivity of a dilute gas of polyatomic molecules and correlated it with the specific heat ratio.
The approximation of Ubbelohde [8]	He considered that molecules of dilute gas in different energy states could be considered as chemical species, which a flux of energy is due to the diffusion of these species.
Theory of Enskog [9]	Enskog made the first important contribution to calculating conductivity of a dense gas by considering the case of hard spheres.
Theory of Longuet-Higgins and Pople [10]	Longuet-Higgins and Pople have calculated conductivity of a dense gas of rigid spheres assuming the existence of a collisional mechanism alone.
Theory of Horrocks and McLaughlin [11,12]	They suggested conductivity in terms of frequency and assuming face-centered cubic lattice geometry.
Theory of Longuet-Higgins and Valleau [13]	They considered that the molecules interact with a square-well potential.
Theory of Davis et al. [14]	Davis et al. carried out a more elaborate treatment of the transport properties of a square-well fluid computing both the convective and collisional contribution on the basis of a modified Boltzmann equation.
Theory of Sengers [15]	His treatment includes the effect of the perturbation of the distribution function from the local equilibrium value which was omitted by Longuet-Higgins and Valleau.
Choh and Uhlenbeck [16], Cohen [17] and Bogolubov [18]	In general, these theories are based on density expansions of a generalized Boltzmann equation, and yield expressions for conductivity in terms of a series expansion in the density.
Second category	
Misic and Thodos [19,20]	For pure component, low pressure (<350 kPa) hydrocarbon gases, they recommend two correlations. One of them for methane and cyclic compounds below reduced temperatures of 1.0, and another for these hydrocarbons above reduced temperatures of 1.0 and for other hydrocarbons at any temperature.
Bromley and Wilke [21]	For pure non-hydrocarbon monatomic gases at low pressure (up through 1 atm).
Bromley and Wilke [21]	For pure non-hydrocarbon linear molecules gases at low pressure (up through 1 atm).
Stiel and Thodos [22]	For pure non-hydrocarbon nonlinear molecules gases at low pressure (up through 1 atm).
Mao-Gang He et al. [23]	They suggested a new correlation to estimate the thermal conductivity of the dense fluid for halogenated hydrocarbon refrigerants.
Edward F. Pliński [24]	He recommended a correlation to estimate thermal conductivity of CO_2, N_2, He, Xe, CO, O_2 and Ar as a function of temperature.

2.1. Artificial neural networks

The concept of neural network models (NNMs) appears to be a recent development. However, this field was established before the advent of computers in attempts to replicate the learning capabilities of biological neural systems by modeling the low-level structure of the brain. Neural networks are computational systems, either hardware or software, which mimics the computational abilities of biological systems by using numbers of simple interconnected artificial neurons [25].

A neural network consists of numbers of simple processing elements called neurons. Each neuron of the neural network is connected to others by means of direct communication links, each with an associated weight, which represents information being used by the network to solve the problem. The output of a neuron is computed from the following equation:

$$O_j = f\left(\sum_{i=1}^{n} w_{ji}x_i + b_j\right) \tag{1}$$

where O_j = output of jth neuron, f = activation or transfer function, b_j = bias of jth neuron, w_{ji} = synaptic weight corresponding to ith synapse of jth neuron, x_i = ith input signal to jth neuron, n = number of input signals to jth neuron.

As Eq. (1) shows bias is an activation threshold added to the product of input data and their respective weighting factors. The most commonly used activation or transfer functions that work well are logarithmic sigmoid, hyperbolic tangent sigmoid and linear functions. Weighted sum of all input plus the bias of neuron

will become the input of activation function. It should be noted that an important characteristics of the activation function is its differentiability, since it facilitates the training of the network through gradient-based training algorithms. The activation function serves mainly as a type of filter or gate that lets some signals move forward and stops others as they progress from the input nodes to the output nodes. Thus, the smaller the value of the neuron's output is, the less its effect on the next neurons would be. There are several types of ANN's such as feedforward network, radial basis function network, ART network and auto associative network [26]. Conventional feedforward networks are the most commonly used one for the function approximation. Hence, the network used in this study is of this type. Multi-layer feedforward networks consist of groups of interconnected nodes arranged in layers corresponding to input layer, hidden and output layers.

The input layer receives all input signals and dispatches them to other neurons. Network's outputs which are provided by the neurons in the output layer are actually the final results of the neuromorphic model. Consequently, number of nodes for the input and output layers are defined by the number of independent and dependent variables, respectively. The input layer is fed with input variables and passes them into the hidden layer(s) where the processing task takes place. Finally, the output layer receives the information from the last hidden layer and sends the results to an external source. The network can therefore be interpreted as a form of input/output model, whose parameters are synaptic weights and biases. This type of network is able to approximate almost all types of functions regardless of their complexities [26].

During the training algorithm, input data are fed to the input layer of the network and the difference between the output layer results and the desired outputs (i.e., network error) is used as a criterion for adjustment of network's synaptic weights and biases. At the beginning, all synaptic weights and biases are initialized randomly. Then, the network is trained (i.e., its synaptic weights are adjusted) by an optimization algorithm until it correctly emulates the input/output mapping.

Selecting the minimum number of data points required to train the neural network is frequently a difficult task, a heuristic guideline states that the number of data points should be 10 times as connections in the network [27]. The optimal network architecture for a specific problem is achieved through a trial and error procedure, in which the structure of the network is changed and the resulting network is trained in such a way that the average root mean square (RMS) error is minimized. The structure of the network can be changed through varying the number of hidden layers as well as the number of neurons in each hidden layer. According to Cybenko [28], a network that has only one hidden layer is able to approximate almost any type of nonlinear mapping. However, the determination of the approximate number of nodes for the hidden layer is difficult, and is often done by trial and error. Too few neurons in the hidden layer impair the network and prevent the network to get trained appropriately. On the other hand, too many nodes allow the network to memorize the pattern (i.e., develop a correlation) presented without capturing the underlying relationship between the input and output variables. These problems that occur during neural network training is called "overfitting". In this case, the error on the training set gets a very small value, but when the network is exposed to new data leads to unacceptably large errors. In other words, the network has memorized the training examples, but it has not learned to generalize. In order to let the network to get trained with sufficient generalizability, the available data should be divided into three subsets. The first subset is the training set, which is used to train the network (i.e., determination of the optimum values of synaptic weight and biases). The second subset is the validation set; the error on the validation is monitored during the training process. The validation error will normally decrease during the initial phase of training and so does the error corresponding to the training data set. However, when the network begins to overfit the data, the error on the validation set will typically begin to rise. When the validation error increases for specified number of iterations, the training is stopped. The weights and biases corresponding to minimum validation and training errors are considered as the optimum values of the synaptic weights and biases. The third subset is the testing data set; this set of data, which is not used during the training, is used to obtain the overall accuracy of the network and to compare the performance of various network structures.

Table 2
List of Compounds used in the development of the neuromorphic model

No.	Component type	No. of data points	T_c	P_c	MW
1	Acetone	6	508.1	46.4	58.08
2	Acetylene	9	308.3	61.4	26.038
3	Ammonia	11	405.6	112.8	17.031
4	Argon	10	150.8	48.7	39.948
5	Benzene	8	562.05	48.95	78.114
6	Bromine	3	584.1	103.0	159.808
7	Carbon dioxide	22	304.2	73.8	44.01
8	Carbon disulfide	2	552.0	78.0	76.131
9	Carbon tetrachloride	5	556.4	45.0	153.823
10	Chlorine	5	417.0	76.0	70.906
11	Chloroform	3	536.4	54.0	119.378
12	Cyclohexane	1	553.5	40.73	84.161
13	Deuterium	3	38.4	16.4	4.032
14	Ethane	6	305.32	48.72	30.07
15	Ethyl acetate	3	523.2	38.3	88.11
16	Ethyl chloride	4	460.4	52.0	64.515
17	Helium	15	5.2	2.27	4.003
18	Heptane	5	540.2	27.4	100.204
19	Hexene	2	504.0	31.43	84.161
20	Hydrogen	15	33.2	13.0	2.016
21	Krypton	3	209.4	55.0	83.8
22	Methane	8	190.6	46.0	16.043
23	Methyl alcohol	2	512.64	80.97	30.042
24	Methylene chloride	4	378.0	61.5	84.9
25	n-Butane	4	425.12	37.96	58.123
26	Neon	5	44.4	27.6	20.183
27	Nitric oxide	3	180.0	65.0	30.006
28	Nitrogen	14	126.2	33.9	28.013
29	Nitrous oxide	2	309.6	72.4	44.013
30	n-Pentane	4	469.7	33.7	72.15
31	Oxygen	12	154.6	50.5	31.999
32	Propylene	5	364.9	46.0	42.081
33	R 11 (Trichlorofluoromethane)	2	471.1	44.72	137.368
34	R 12 (Dichlorodifluoromethane)	6	385.1	41.3	120.913
35	R 13 (Chlorotrifluoromethane)	4	302.0	38.7	104.459
36	R 22 (Chlorodifluoromethane)	4	369.28	49.86	86.468
37	Sulfur dioxide	5	430.8	77.8	64.063
38	Water vapor	8	647.3	220.5	18.015
39	Xenon	3	289.7	58.4	131.3
	Total	236			

2.2. Data acquisition and analysis

Perhaps one of the most important decisions in the development of the neuromorphic model is availability of reliable experimental sources of data for the model. A set of 236 experimental data points for hydrocarbon and non-hydrocarbon compounds was used to develop the neuromorphic model. These data include experimental published data on critical temperature, critical pressure, molecular weight and thermal conductivity for pure components [29–39]. The data set used in the development of the neuromorphic model contains both hydrocarbon and non-hydrocarbon compounds of various types shown in Table 2. Table 3 summarizes the overall range of experimental data points used in the development of the multi-layer perceptron network proposed in this work. Although there are more data points available in open literature,

Table 3
Range of pure components properties

Property	Minimum	Maximum
Temperature (K)	90.2	2000
Critical temperature (K)	5.20	647.3
Critical pressure (bar)	2.27	220.5
Molecular weight	2.016	159.808
Conductivity (W/m°C)	0.0038	0.412

since some of them are not obtained through experimental measurement and are the results of estimation, they were excluded from the data points used in this study.

After identifying and collecting the data set, the next step is the selection of input variables, which are model's independent variables. The available correlations for prediction of conductivity at constant pressure are essentially based on the assumption that conductivity can be described as a function of temperature, critical temperature, critical pressure and molecular weight as follows:

$$k = f(T, T_c, P_c, MW) \tag{2}$$

Following this approach, temperature, critical temperature, critical pressure and molecular weight were used as the inputs of the ANN model for the prediction of conductivity for pure gases.

2.3. Neural network training

Once the input data have been selected, the next step is to develop the artificial neural network architecture; a network with only one hidden layer was selected as the starting network structure. In order to find the number of neurons in the hidden layer a constructive approach was used [40]. Based on the constructive approach, a small number of neurons are used in the hidden layer and if the error of the trained network does not meet the desired tolerance the number of neurons in the hidden layer is increased by one and training cycle and performance evaluation is repeated. This procedure is continued until the trained network performs satisfactorily (i.e., its training, validation and testing errors are lower than the target goal).

The feedforward network was trained by Levenberg Marquardt algorithm [41–43]. Applying the constructive approach to design the neural network model for the estimation of conductivity led to a three-layer network with four neurons in input layer, eight neurons in hidden layer and one neuron at output layer.

2.4. Selection of optimal configuration

The performance of a trained network can be measured to some extent by the errors on the training, validation and test data sets, but it is often useful to investigate the network response in more detail. Regression analysis was done to assess the network capability for conductivity prediction. The coefficient of determination, R^2, was used as a measure to evaluate how the trained network estimation is compatible to the experimental data.

Also, different neural network topologies were compared using their mean relative errors (MRE) and mean square errors (MSE). The MRE and MSE are defined with the following equations:

$$\mathrm{MRE} = \frac{1}{N}\sum_{i=1}^{N}\frac{|k_{\exp} - k_p|}{k_{\exp}} \tag{3}$$

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(k_{\exp} - k_p)^2 \tag{4}$$

N is the number of data points, and $k_{\exp}$ and k_p are the experimental and predicted values of thermal conductivity, respectively.

Table 4
The MRE, MSE and R values for the different neural network configurations

No. of neurons	MRE	MSE	R-value
5	9.5299	1.2079×10^{-5}	0.9986
8	7.4339	7.5283×10^{-6}	0.9991
10	5.4241	3.8302×10^{-6}	0.9996
12	5.7747	3.9396×10^{-6}	0.9996
15	7.3112	6.3613×10^{-6}	0.9993
20	8.6723	1.4370×10^{-5}	0.9983

3. Results and discussion

Table 4 shows the MRE, MSE and R values calculated for various neural network configurations differing with respect to their number of hidden layer neurons. The configuration with minimum error measures (i.e., MRE and MSE), and appropriate R-value, was selected as the best network architecture. According to Table 4, the best neural network configuration has one hidden layer with ten neurons. The variation of the training error for the best neural network is presented in Fig. 1.

Fig. 2 illustrates the correlation between the simulation results of the neural network and the experimental training data points. The perfect fit (output equal to targets) is indicated by the solid line. The close proximity of the best linear fit to the perfect fit, as observed in Fig. 2, shows a good correlation among the network predictions and the experimental data.

Also, the performance of the best developed network was tested using another data set consisting of 96 data points not previously used for the network training. The results of the test indicate that the MRE and MSE for the proposed model are about 5.424% and 3.8302×10^{-6}, respectively. Fig. 3 indicates correlation between the predicted and experimental test data of thermal conductivity.

The network outputs with the test data set are plotted versus the targets as stars. The perfect fit (output equal to targets) is indicated by the solid line. The slope and the y-intercept of the best linear regression relating targets to the network outputs are respectively 1.0045 and 1.2269×10^{-4} which nearly overlaps the perfect linear fit. The correlation coefficient (R-value) between the network predictions and the experimental test data is 0.9996. This shows a very good correlation among the simulated and test data.

Table 5 summarizes the results of applying the neural network model and other methods to predict the thermal conductivity of pure gases. Also, the experimental values of conductivities are given in the table for comparison. This table shows that the accuracy of the proposed method is almost more than the accuracy of the other correlations despite the number of input variables required for the proposed method is less than that of most other alternative methods. While some of gases shown in the table were not used in the training, we applied the proposed neural network to them to assess the extrapolation capability of the model. It should be notified that there is no unique correlation to estimate thermal conductivities over the wide range of components and temperatures given in Table 5. Therefore, based on the component type and temperature range, the best correlations were selected in each case to predict the conductivities to be compared with the network model estimates.

Indeed, one of important advantage of the developed ANN model is that a single trained ANN can cover a wide range of temperature and molecular types of gases while other proposed correlations have some limitations with this respect. The correlations reported in the literature are valid only for specific gases. For instance, for pure non-hydrocarbon monatomic gases and non-hydrocarbon linear molecules at low pressure (up to 1 atm), Bromley [21] suggested two distinct correlations to predict the gas thermal conductivity. Also, Stiel and Thodos [22] presented a correla-

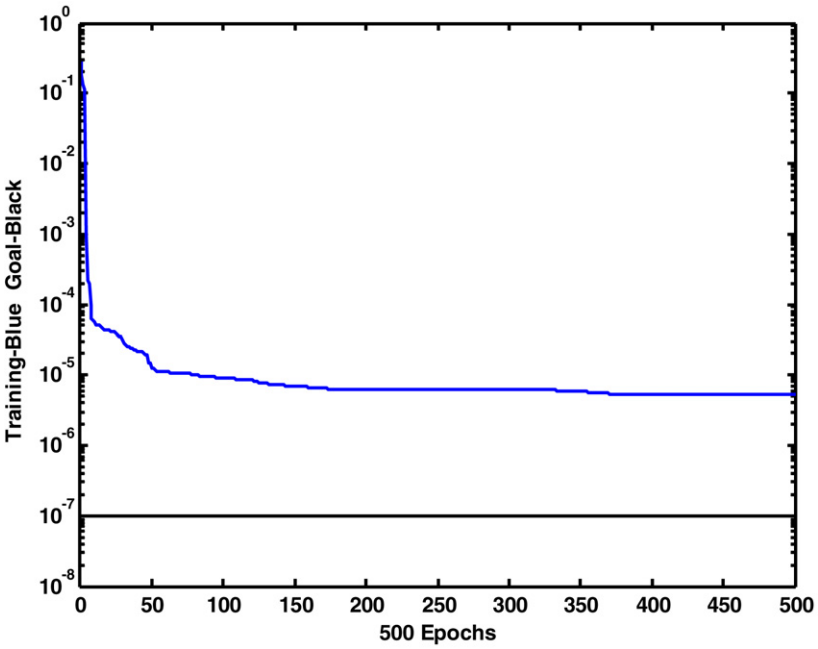

Fig. 1. A schematic of error variation during training.

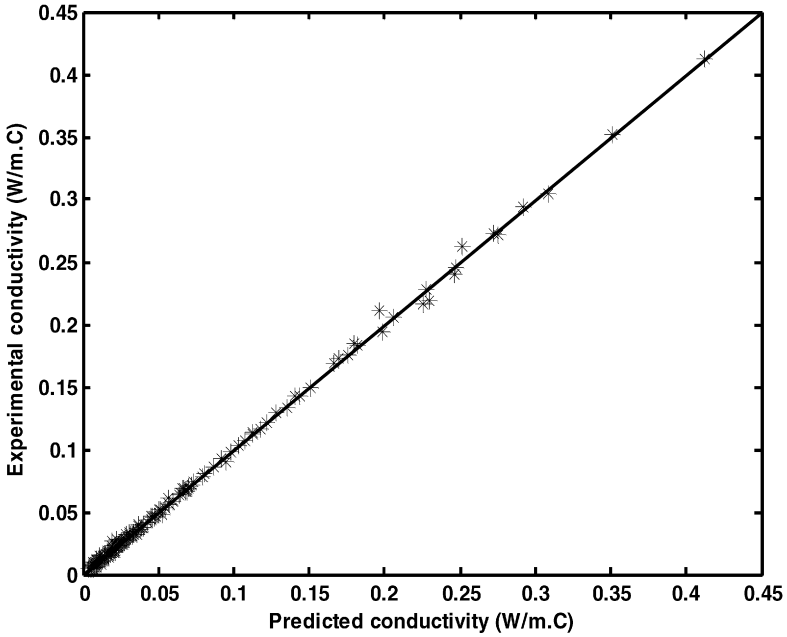

Fig. 2. Correlation of experimental data versus neural network predictions for training data set.

tion for pure non-hydrocarbon nonlinear molecules at low pressure (up to 1 atm). These correlations have higher average errors for polar compounds (e.g., ammonia, sulfur dioxide and water vapor in Table 5). These correlations, in addition to temperature, critical temperature, critical pressure and molecular weight, require accurate values for the heat capacity at constant volume and also vapors viscosity which is usually not available for compounds at any temperature (e.g., carbon dioxide at 1500 K and carbon monoxide at 81.88 and 91.88 K in Table 5). Misic and Thodos [19,20] recommended two correlations for pure component, low pressure ($<$350 kPa) hydrocarbon gases. One of their correlations has been proposed for methane and cyclic compounds below reduced temperatures of 1.0, and the other one has been recommended for all hydrocarbons above reduced temperatures of 1.0. These correlations, in addition to the input data needed for the neural network model, requires the heat capacity at constant pressure. The Artificial Neural Network (ANN) model proposed in this article is based on the critical temperature, critical pressure and molecular weight that is available for all gases. This is one of the advantages of the ANN model with respect to other correlations.

4. Conclusions

A neural network based model was developed for the prediction of thermal conductivity of pure gases at atmospheric pressure as a function of temperature. The model input variables are temperature, molecular weight, critical pressure and temperature. The best architecture of the feedforward network, obtained by trial and

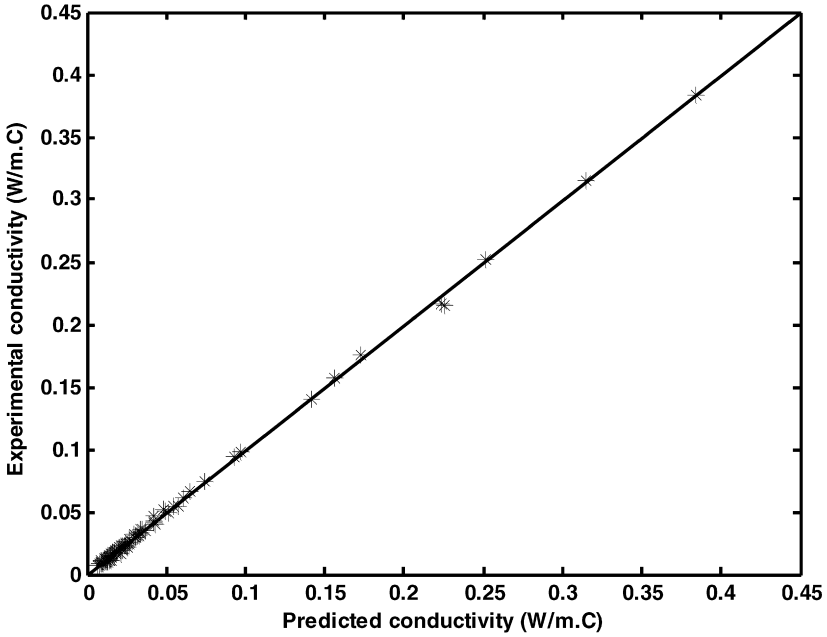

Fig. 3. Correlation of experimental data versus neural network values of thermal conductivity for the test data set.

Table 5
Comparison of the proposed ANN model with experimental data and other correlations

No.	Compound	Temp. (K)	Experimental conductivity (W/m °C)	The ANN prediction (W/m °C)	RE (%)	Other correlations (W/m °C)	RE (%)
1	Acetone	300	0.0115	0.0125	8.69	0.0101[2]	12.17
		400	0.0201	0.0211	4.97	0.0187[2]	6.96
2	Acetylene	293	0.0218	0.0206	5.50	0.0213[2]	2.29
		400	0.0332	0.0333	0.30	0.0332[2]	0.00
3	Ammonia	353	0.0301	0.0292	2.99	0.0355[5]	17.94
		400	0.0364	0.0346	4.94	0.0424[5]	16.48
4	Argon	273.2	0.0163	0.0173	6.13	0.0166[3]	1.84
		491.2	0.0267	0.0280	4.86	0.0265[3]	0.74
5	Benzene	319.11	0.0126	0.0127	0.79	0.0118[2]	6.34
		400	0.0195	0.0199	2.05	0.0189[2]	3.07
6	Carbon dioxide	273.1	0.0146	0.0148	1.36	0.0147[4]	0.68
		400	0.0246	0.0249	1.21	0.0248[4]	0.81
		473	0.0313	0.0305	2.55	0.0306[4]	2.23
		600	0.0431	0.0398	7.65	0.0402[4]	6.77
		1100	0.0744	0.0738	0.80	0.0835[4]	12.23
		1500	0.0974	0.0980	0.61	[6]	
7	Carbon monoxide[1]	81.88	0.0071	0.0071	0.00	[6]	
		91.88	0.0080	0.0079	1.25	[6]	
		273	0.0221	0.0222	0.45	0.0237[4]	7.23
		291	0.0237	0.0236	0.42	0.0249[4]	5.06
8	Carbon tetrachloride	319.11	0.0071	0.0067	5.63	0.0072[5]	1.40
		456.88	0.0112	0.0124	10.71	0.0111[5]	0.89
9	Chlorine	300	0.0089	0.0097	8.98	0.0084[4]	5.61
10	Chloroform	319.11	0.0080	0.0071	11.25	0.0071[2]	11.25
11	Ethane	239.11	0.0149	0.0142	4.69	0.0144[2]	3.35
		300	0.0218	0.0217	0.45	0.0214[2]	1.83
		500	0.0516	0.0496	3.87	0.0509[2]	1.35
12	Ethyl alcohol[1]	293	0.0154	0.0106	31.16	0.0112[2]	27.27
		373	0.0215	0.0167	22.32	0.0193[2]	10.23
13	Ethylene[1]	250	0.0152	0.0167	9.86	0.0150[2]	1.31
		273	0.0183	0.0196	7.10	0.0174[2]	4.91
		300	0.0214	0.0230	7.47	0.0203[2]	5.14
		400	0.0342	0.0365	6.72	0.0329[2]	3.80
		500	0.0491	0.0509	3.66	0.0468[2]	4.68
		600	0.0653	0.0668	2.29	0.0615[2]	5.81
14	Helium	144	0.0928	0.0947	2.04	0.1059[3]	14.11
		273.2	0.1418	0.1401	1.19	0.1456[3]	2.67
		373.2	0.1731	0.1754	1.32	0.1807[3]	4.39
		489	0.2250	0.2155	4.22	0.2181[3]	3.06

(*continued on next page*)

Table 5 (*Continued*)

No.	Compound	Temp. (K)	Experimental conductivity (W/m °C)	The ANN prediction (W/m °C)	RE (%)	Other correlations (W/m °C)	RE (%)
15	Heptane	300	0.0120	0.0112	6.66	0.0107[2]	10.83
		500	0.0325	0.0308	5.23	0.0327[2]	0.61
16	Hexane[1]	273	0.0125	0.0103	17.6	0.0093[2]	25.6
		298	0.0138	0.0119	13.76	0.0117[2]	15.21
17	Hydrogen	250	0.1561	0.1574	0.83	0.1604[4]	2.75
		373	0.2233	0.2166	3.00	0.2156[4]	3.44
		450	0.2510	0.2513	0.11	0.2418[4]	3.66
		600	0.3150	0.3148	0.06	0.2968[4]	5.77
		800	0.3840	0.3839	0.02	0.3744[4]	2.50
18	iso-Butane[1]	273	0.0138	0.0140	1.44	0.0130[2]	5.79
		373	0.0241	0.0229	4.97	0.0248[2]	2.90
19	iso-Pentane[1]	273	0.0125	0.0121	3.20	0.0110[2]	12.00
		373	0.0220	0.0195	11.36	0.0221[2]	0.45
20	Krypton	491.2	0.0145	0.0153	5.51	0.0149[3]	2.75
21	Methane	200	0.0218	0.0221	1.37	0.0207[2]	5.04
		300	0.0343	0.0361	5.24	0.0322[2]	6.12
		400	0.0484	0.0517	6.81	0.0464[2]	4.13
22	Methyl acetate[1]	273	0.0102	0.0091	10.78	0.0081[2]	20.58
		293	0.0118	0.0102	13.55	0.0097[2]	17.79
23	Methyl chloride[1]	273	0.0092	0.0111	20.65	0.0088[2]	4.34
		319.11	0.0125	0.0135	8.00	0.0117[2]	6.40
		373	0.0163	0.0167	2.45	0.0154[2]	5.52
		456.88	0.0225	0.0225	0.00	0.0215[2]	4.44
		484.66	0.0256	0.0247	3.51	0.0236[2]	7.81
24	n-Butane	273	0.0135	0.0136	0.74	0.0128[2]	5.18
		400	0.0264	0.0246	6.81	0.0280[2]	6.06
25	Neon	373.2	0.0580	0.0550	5.17	0.0470[3]	18.96
26	Nitric oxide	200	0.0186	0.0162	12.90	0.0202[4]	8.60
27	Nitrogen	273	0.0230	0.0231	0.43	0.0242[4]	5.21
		400	0.0333	0.0325	2.40	0.0326[4]	2.10
		900	0.0607	0.0613	0.98	0.0651[4]	7.24
28	Nitrous oxide	273	0.0159	0.0146	8.17	0.0152[5]	4.40
29	n-Pentane	273	0.0128	0.0118	7.81	0.0108[2]	15.62
		293	0.0144	0.0131	9.02	0.0128[2]	11.11
30	Oxygen	173	0.0164	0.0164	0.00	0.0189[4]	15.24
		200	0.0182	0.0185	1.64	0.0195[4]	7.14
		350	0.0307	0.0304	0.97	0.0298[4]	2.93
		500	0.0417	0.0409	1.91	0.0414[4]	0.71
31	Propane[1]	250	0.0129	0.0131	1.55	0.0121[2]	6.20
		273	0.0151	0.0153	1.32	0.0146[2]	3.31
		300	0.0183	0.0180	1.63	0.0177[2]	3.27
		373	0.0261	0.0258	1.14	0.0271[2]	3.83
		400	0.0295	0.0289	2.03	0.0309[2]	4.74
		500	0.0417	0.0418	0.23	0.0455[2]	9.11
32	R 12	300	0.0097	0.0095	2.06	0.0094[5]	3.09
		373	0.0138	0.0125	9.42	0.0125[5]	9.42
33	R 21[1]	300	0.0088	0.0082	6.81	0.0082[2]	6.81
		400	0.0135	0.0122	9.62	0.0134[2]	0.74
		500	0.0181	0.0171	5.52	0.0186[2]	2.76
34	R 22	400	0.0170	0.0179	5.29	0.0169[2]	0.58
35	Sulfur dioxide	273	0.0087	0.0087	0.00	0.0096[5]	10.34
		373	0.0119	0.0118	0.84	0.0144[5]	21.00
36	Water vapor	353	0.0218	0.0233	6.88	0.0275[5]	26.14
		450	0.0299	0.0293	2.00	0.0407[5]	36.12
		600	0.0422	0.0424	0.47	0.0573[5]	35.78
		750	0.0549	0.0547	0.36	0.0767[5]	39.70
37	Xenon	491.2	0.0093	0.0114	22.58	0.0083[3]	10.75

[1] Not used in the training of the proposed ANN.
[2] The correlation of Misic and Thodos [19,20].
[3] The correlation of Bromley for pure non-hydrocarbon monatomic gases [21].
[4] The correlation of Bromley for non-hydrocarbon linear molecules [21].
[5] The correlation of Stiel and Thodos [22].
[6] The vapors viscosity is not available for these compounds at given temperature.

error, consists of one hidden layer with ten neurons. Application of the proposed ANN model to the training and test data indicates that it is able to predict thermal conductivity of pure gases with a considerably lower relative error than that of other alternative correlations. Also, it should be mentioned that the number of input required data of the ANN method is less than most other proposed correlations. On the other hand, the correlations suggested in the literature have some limitation with respect to applicable temperature range and the gas molecular structure. But the ANN model developed in this work is not suffered from such constraints. The results of applying the trained neural network model to the test data indicate that the method has a very good interpolation and

extrapolation capabilities with respect to not only the temperature ranges but also the molecular types.

References

[1] I.J. Turias, J.M. Gutiérrez, P.L. Galindo, Modeling the effective thermal conductivity of an unidirectional composite by the use of artificial neural networks, Composites Science and Technology 65 (2005) 609–619.
[2] S.S. Sablani, R.M. Shafiur, Using neural networks to predict thermal conductivity of food as a function of moisture content, temperature, and apparent porosity, Food Research International 36 (2003) 617–623.
[3] S.S. Sablani, O.-D. Bike, M. Marcotte, Neural networks for predicting thermal conductivity of bakery products, Journal of Food Engineering 52 (2002) 299–304.
[4] N. Therdthai, W. Zhou, Artificial neural network modeling of the electrical conductivity property of recombined milk, Journal of Food Engineering 50 (2001) 107–111.
[5] M. Jalali-Heravi, M.H. Fatemi, Prediction of thermal conductivity detection response factor using an artificial neural networks, Journal of Chromatography 897 (2000) 227–235.
[6] S. Chapman, T.G. Cowling, The Mathematical Theory of Non-Uniform Gases, Cambridge University Press, London, 1953.
[7] J.O. Hirschfelder, R.B. Bird, The Molecular Theory of Gases and Liquids, Wiley, New York, 1954.
[8] A.R. Ubbelohde, The thermal conductivity of polyatomic gases, J. Chem. Phys. 3 (1935) 219.
[9] R.P. Tye, Thermal Conductivity, vol. 2, Academic Press, London/New York, 1969.
[10] H.C. Longuet-Higgins, J.A. Pople, Transport properties of a dense fluid of hard spheres, J. Chem. Phys. 25 (1956) 884.
[11] J.K. Horrocks, E. McLaughlin, Non-steady-state measurements of the thermal conductivities of liquid polyphenyls, Proc. R. Soc. 273 (1963) 259.
[12] J.K. Horrocks, E. McLaughlin, Trans. Faraday Soc. 59 (1963) 1709.
[13] H.C. Longuet-Higgins, J.P. Valleau, Transport coefficients of dense fluids of molecules interacting according to a square well potential, Molec. Phys. 1 (1958) 284.
[14] H.T. Davis, S.A. Rice, J.V. Sengers, On the kinetic theory of dense fluids. IX. The fluid of rigid spheres with a square-well attraction, J. Chem. Phys. 35 (1961) 2210–2233.
[15] J.V. Sengers, Divergence in the density expansion of the transport coefficients of a two-dimensional gas, Phys. Fluids 9 (1966) 1685–1696.
[16] S.T. Choh, G.E. Uhlenbeck, The kinetic theory of phenomena in dense gases, University of Michigan Report, 1958.
[17] E.G.D. Cohen, in: J. Meixne (Ed.), Statistical Mechanics of Equilibrium and Non-equilibrium Processes, North-Holland, Amsterdam, 1965.
[18] G.N.N. Bogolubov, in: J. de Boer, G.E. Uhlenbeck (Eds.), Studies in Statistical Mechanics, vol. 7, North-Holland, Amsterdam, 1962.
[19] D. Misic, G. Thodos, Thermal conductivity of hydrocarbon gases at normal pressures, AIChE J. 7 (1961) 264.
[20] D. Misic, G. Thodos, Atmospheric thermal conductivity for gases of simple molecular structure, J. Chem. Eng. Data 9 (1963) 540.
[21] L.A. Bromley, Thermal conductivity of gases at moderate pressures, University of California Radiation Laboratory, Report No. UCRL-1852, Berkeley, CA, 1952.
[22] L.I. Stiel, G. Thodos, AIChE J. 10 (1964) 26–32.
[23] M.-G. He, Z.-G. Liu, J.-M. Yin, New equation of state for transport properties: calculation for the thermal conductivity and viscosity of halogenated hydrocarbon refrigerants, Fluid Phase Equilibrium 201 (2002) 309–320.
[24] E.F. Pliński, J.S. Witkowski, Prediction of the thermal properties of CO2, CO, and Xe laser media, Optics & Laser Technology 32 (2001) 61–66.
[25] M.T. Hagan, H.B. Demuth, M.H. Beale, Neural Network Design, PWS Publishing, Boston, MA, 1996.
[26] R. Boozarjomehri, F. Abdolahi, M.A. Moosavian, Characterization of basic properties for pure substances and petroleum fractions by neural network, Fluid Phase Equilibria 231 (2005) 188–196.
[27] Statistical Neural Networks, User's Manual, Release 4.0 F, Statsoft, Tulsa, OK, 2000.
[28] G.V. Cybenko, Mathematics of control, Signals Syst. 2 (1989) 303–314.
[29] R.H. Perry, D.W. Green, Perry's Chemical Engineers Handbook, seventh ed., McGraw-Hill, 1997.
[30] R.C. Reid, J.M. Prausnitz, B.E. Poling, The Properties of Gases and Liquids, fourth ed., McGraw-Hill, New York, 1987.
[31] J.P. Holman, Heat Transfer, eighth ed., McGraw-Hill, United States of America, 1997.
[32] D. Robert, Thermal Conductivity of Gases and Liquids, MIT Press, Cambridge, MA, 1965.
[33] B.G. Dickens, Proc. Roy. Soc. (London) A 143 (1934) 517.
[34] A. Eucken, On the temperature dependence of the thermal conductivity of some gases, Physik Z. 12 (1911) 1101–1107 (in German).
[35] H. Gregory, S. Marshall, Thermal conductivities of oxygen and nitrogen, Proc. Roy. Soc. (London) A 118 (1928) 594–607.
[36] E.W. Washburn (Ed.), International Critical Tables, McGraw-Hill, New York, 1929.
[37] W.B. Mann, B.G. Dickens, Proc. Roy. Soc. (London) A 134 (1931) 77.
[38] E. Moser, Dissertation, Berlin, 1913.
[39] G.G. Sherratt, E. Griffiths, A hot-wire method for the thermal conductivity of gases, Phil. Mag. 27 (1939) 68.
[40] S. Haykin, Neural Networks: A Comprehensive Foundation, second ed., Prentice-Hall, Englewood Cliffs, NJ, 1999.
[41] K. Levenberg, A method for the solution of certain problems in least squares, SIAM J. Numer. Anal. 16 (1944) 588–604.
[42] D. Marquardt, An algorithm for least-squares estimation of nonlinear parameters, SIAM J. Appl. Math. 11 (1963) 431–441.
[43] M.T. Hagan, M. Menhaj, IEEE Trans. Neural Netw. 5 (1994) 989–993.