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Developing Genetic Algorithm-Based Neural Networks and the Sensitivity Analysis for the Thermal Conductivity of Natural Gases

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ABSTRACT

The artificial neural network (ANN) approach was applied to develop simple correlations for predicting the thermal conductivity of nitrogen-methane and carbon dioxide-methane mixtures. The genetic algorithm method was used to obtain global optimum parameters (weights and biases) of the ANNs. The methane mole fraction, temperature, pressure, and density as effective parameters on the thermal conductivity were network input variables. 171 and 180 data points related to the nitrogen-methane and carbon dioxide-methane gas mixtures respectively, divided to test and train datasets. Simple correlations were obtained due to the small number of optimal neurons in the ANN structures. The mean relative errors of 0.206 % and 0.199 % for the testing dataset indicate the high accuracy and validation of the correlations. The work indicates that artificial intelligence approaches are very useful for the thermal conductivity modeling in natural gases. A sensitivity analysis was performed on all input variables that indicates that the gas mixture density has the greatest impact on the thermal conductivity.

1. Introduction

The thermal conductivity of a gas mixture directly affects the modeling and designing of heat transfer systems. On the other side, the heat transfer phenomenon is the main process in such practical applications of chemical engineering as heat exchangers, power plants, and steam generators [1, 2]. The measurement of the thermal conductivity of all possible combinations of all mixtures is not practical. Therefore, developing accurate and simple predictive correlations is very suitable.

There are relatively rare precise measurements and models for the thermal conductivity of binary mixtures containing the natural gas components including methane, ethane, propane, nitrogen, and carbon dioxide. Patek et al. [3] measured the thermal conductivity of gas mixtures of carbon dioxide and methane at temperatures between 300 and 425 K and pressures up to 12 MPa at three mole fractions of methane. The results related to the low-density analysis of the experimental data were employed to investigate the estimation of the thermal conductivity of nonpolar mixtures for the dilute-gas limit proposed in the literature [4]. Moreover, the thermal conductivity of gas mixtures of nitrogen and methane at temperatures between 300 and 425 K and at pressures up to 16 MPa were investigated by Patek et al. [5]. The measured experimental

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data have been obtained using transient hot-wire instruments [6].

The artificial neural network (ANN) model as a subset of the artificial intelligence (AI) was applied widely in various fields of engineering over the last two decades. Panerati et al. [7] reviewed the application of ANNs such as modeling, classification, and prediction in chemical engineering. Pirdashti et al. [8] investigated the ANN application in the environmental, health and safety and nanotechnology fields and so on. Moreover, the ANNs are powerful techniques for solving problems related to the physical and thermodynamic properties such as viscosity, the diffusion coefficient, the thermal conductivity, etc. The diffusion coefficients in binary liquid [9] or gas mixtures [10], and the critical temperature and pressure of binary hydrocarbon mixtures [11] were modeled using neural network techniques. Ghaderi et al. [12] developed ANNs for predicting the fluid viscosity in different density ranges. They concluded that ANN had suitable accuracy in high densities while other investigated computational techniques were inappropriate for the density of more than 8. Fazlali et al. [13] investigated the ANN model for estimating vapor-liquid equilibrium data for mixtures of water, ethanol and 1-butyl-3-methylimidazolium acetate. The prediction performance was compared with the performace of the non-random-two-liquid (NRTL) and electrolyte non-random-two-liquid (eNRTL) approaches. They proved the superiority of the neural network. Eslamloueyan and Khademi [14] developed ANNs for the prediction of thermal conductivity of pure gases in atmospheric pressure as a function of the critical temperature, critical pressure, and molecular weight.

The combination of the neural network and genetic algorithm (GA) can lead to an increased ANN capability. The GA indicates the natural selection procedure in which the most appropriate people are selected to reproduce next generation children [15, 16]. In the ANN-GA modeling procedure, the genetic algorithm search technique was used to obtain the suitable parameters of the ANN. The improved performance for this compound has been reported in the literature [17]. Beigzadeh et al. [18] used the ANN-GA for predicting the heat transfer and pressure loss for the air convection on interrupted plate fins. The employed data for developing the model was acquired using the computational fluid dynamics (CFD). Kumar et al. [19] investigated the combination of GA with ANN and an adaptive network-based fuzzy inference system (ANFIS) for improving and optimizing the process of the biobleaching of the mixed hardwood pulp.

The relation between the properties of natural gas mixture components and the thermal conductivity is complicated. Most models presented in the literature for estimating the thermal conductivity of natural gas are complex and require many parameters. In this study, The ANNs have been used for developing a regression equation to obtain the thermal conductivity of natural gases with a high calculation speed and accuracy. The neural networks can distinguish hidden patterns and nonlinear relationships in raw data points and they typically use a less statistical training process. The study tries to develop simple correlations for predicting the thermal conductivity of the two gas mixtures including nitrogen-methane and carbon dioxide-methane. The developed correlations involving all main and effective parameters include methane mole fraction, temperature, pressure, and density. The study of empirical data revealed a nonlinear relation between input and target variables. The proposed correlations are accurate, simple, and convenient. The validity of the employed models was proved by the test data set that had no role in the neural network training process.

2. Data collection and preprocessing

The first stage to develop the neural network model is collecting sufficient and suitable data points from valid sources to train the ANN. A set of 171 and 180 experimental data points of the thermal conductivity of nitrogen-methane and carbon dioxide-methane mixtures respectively, was applied to train the neuromorphic model. Such experimental data is mainly achieved from the experimental measurement reported in Refs. [3, 5]. The experiments have been made by means of transient hot-wire instruments as explained in detail in Ref. [6]. The ANN model requires a lot of data points for a high prediction accuracy. The suitable data points related to the thermal conductivity of nitrogen-methane and carbon dioxide-methane mixtures were found in the used Refs. [3, 5]. The high prediction accuracy for the developed ANN models indicates the ability of the model for other natural gas mixtures.

In the present work, the ANN input data have been methane mole fraction, temperature, pressure, and the density of the investigated gas mixtures. The ANN models were developed with and without the density and it was observed that the use of density as the input variable improved the model accuracy. All input-output data points were divided randomly into two categories including training (70 %) and testing (30 %) data sets. Table 1 presents the ranges of data points used in this research to develop the ANN model. All input and output data were normalized due to the different ranges of the employed data and to expedite the process of neural network training. All dependent and independent variables were within the normal range of 0-1 to prevent any difficulties. The calculation is as follows:

$$\text{Normalized data} = \frac{\text{data value} - \text{minimum value}}{\text{maximum value} - \text{minimum value}} \tag{1}$$

Table 1
Range of studied variables for models.

Variable	Nitrogen-Methane		Carbon dioxide-Methane	
	Min	Max	Min	Max
x_{CH4}	0.2507	0.7494	0.2493	0.7496
T (K)	300	425	300	425
P (k Pa)	730	15450	724	11970
ρ (mol/m^3)	264.5	6475	297.5	4053
λ (W/m.K)	0.02858	0.05217	0.02096	0.05348

3. Developing ANN-based correlations

The artificial neural network (ANN) as a subset of the artificial intelligence (AI) is related to modeling an intelligent computer structure that has properties like human intelligence. The developed model has the capability of obtaining knowledge and reasoning for solving problems. Due to the limitations of the classic theoretical approaches in practical applications, alternative methods are needed. The ANNs are employed to develop predictive models by their flexible structure based on several parameters (weights and biases).

There are some ANN types in which multilayer feed-forward networks (MFNs) are the most usually used neural networks that are able to estimate nearly all forms of complex nonlinear relationships with a high accuracy [20-22]. There are three main layers in the interconnected structure of the ANN. There are input, hidden, and output layers and they contain one or more neurons. Studies have revealed that one hidden layer is sufficient for an accurate modeling. The input information of the network is transmitted through the input layer toward the hidden and output layers. The final output of the model is calculated as follows:

$$Y=F\left\{\sum_{j=1}^{n} W_{kj}\left[F\left(\sum_{i=1}^{m} W_{ji}X_i+b_j\right)\right]+b_k\right\} \tag{2}$$

where n is the number of hidden neurons, m is the number of input parameters, X is ANN input, the subscripts of "i", "j" and "k" denote the ANN layers, and W and b are the network weights and biases. F is the transfer function to generate the normalized neuron output from the hidden and output layers. Investigations show that the transfer functions of logistic and hyperbolic tangent sigmoids are appropriate for modeling several non-linear problems [23].

The number of neurons in the input and output layers is related to the number of input and output variables respectively. The key step in the development of ANN is to determine the optimal number of neurons in the hidden layer. The process of determining the optimal number of neurons should not result in overfitting [24]. The trial-and-error procedure seems to be the most reliable method for this optimization. In this way, a network error is calculated for a small number of hidden neurons. The number of neurons then increases until the error value does not change or increase.

Two simple correlations were developed using the multi-layer perceptron neural networks to predict the thermal conductivity of nitrogen-methane and carbon dioxide-methane mixtures. During the training of ANN, the parameters (weights and biases), that make the network outputs near to the target data, are determined. The Levenberg-Marquardt back propagation (LM-BP) procedure, in which the network was updated by a specific training design, was used to optimize the weights and biases [25].

3.1. Genetic algorithm

The determination of random initial weights and biases of the ANN is the main weakness of the back-propagation (BP) method which leads to getting trapped in the local minima and slow converging. The genetic algorithm (GA) can overcome the disadvantages by determining the globally optimum values of initial weights and biases [26]. The GA approach is a useful tool for solving the optimization problems. This method is inspired by the principle of Darwinian evolution. The optimization process starts with an initial group of random solutions and progresses with iterations for generations to improve solutions. The operations of selection, crossover, and mutation are the main steps of the GA.

Figure 1 illustrates the flow chart which has been employed in the work and is related to the combined neural network method and genetic algorithm. Generally, the genetic algorithm applied to four stages to acquire the optimal parameters of the ANN [27, 28]:

- Generating the initial population of chromosomes (ANN parameters) randomly.
- Computing the fitness values (deviations) of the ANN.
- Using the selection, crossover and mutation steps to reproduce a new generation.
- Employing a new population in the next generation and if reaching the stopping criteria, the final population of parameters (weights and biases) was being chosen as the GA result.

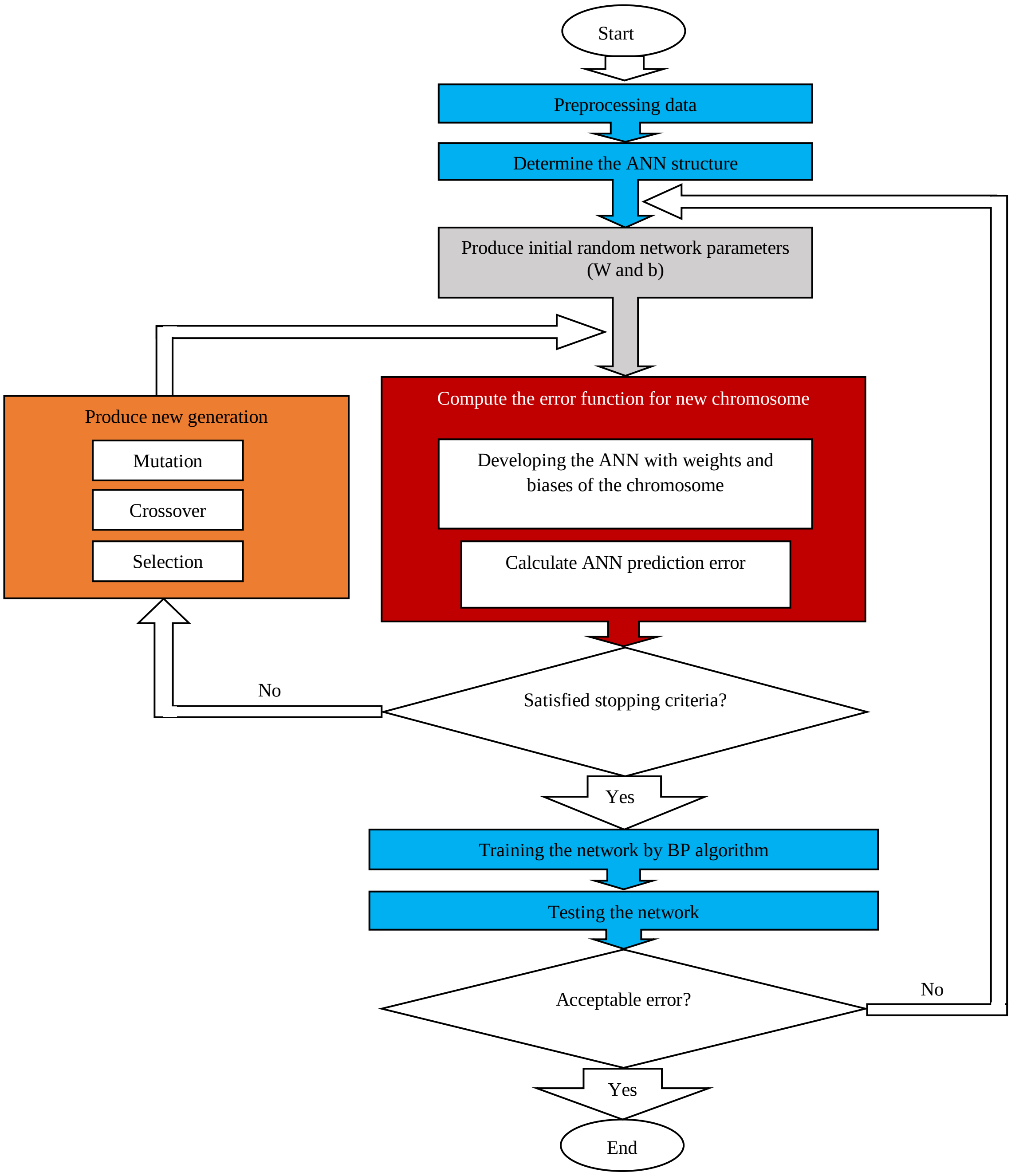


Figure 1. Flow chart for the ANN–GA modeling procedure.

In this study, the numbers of chromosomes in the initial population and in the crossover fraction were selected as 200 and 0.8 respectively. The elite children's number was

1 and the GA would stop after 300 generations (it had practically reached optimum results). In the next step, the BP technique was used to improve the GA results to obtain the optimum solution.

The last stage is validating the performance of the developed model using the testing data. In the work, the mean square error (MSE) and the mean relative error (MRE) between the experimental and target data were applied to evaluate the models, in which N is the total number of data used:

$$\mathrm{MSE}=\frac{1}{N}\sum_{i=1}^{N}(\mathrm{Target}_i\text{-Experimental data}_i)^2 \tag{3}$$

$$\mathrm{MRE}\,(\%)=\frac{100}{N}\sum_{i=1}^{N}\left(\frac{\left|\mathrm{Target}_i\text{-Experimental data}_i\right|}{\mathrm{target}_i}\right) \tag{4}$$

4. Results and discussion

In the present work, it has been attempted to predict the thermal conductivity of two natural gases including nitrogen-methane and carbon dioxide-methane using precise and simple correlations. Two simple correlations were developed by the ANN modeling procedure. The models were trained based on data in the literature at various temperatures, pressures, densities, and methane mole fractions. Ranges of the employed data in the modeling process are shown in Table 1.

The examined neural network comprise one hidden layer in which the appropriate number of neurons was investigated by the trial-and-error method. Trial-and-error is a problem-solving technique in which multiple efforts are made to obtain an answer. This procedure is repeated until getting success (a solution is achieved) and guarantees the optimal number of neurons in the hidden layer. Figure 2 shows the trend of MRE values in terms of the increase in the number of neurons in the hidden layer of the ANN. The performance related to both systems is shown in the figure. It is clear that there is no significant effect on the model performance for more than three hidden neurons. In addition, applying more neurons leads to complicating the model and overfitting [24]. Therefore, ANNs with three neurons were considered as optimum structures. The MRE and MSE values of the developed neural network for predicting the thermal conductivity of nitrogen-methane were 0.157 % and 7.50×10-9 respectively. Moreover, the values of 0.175 % and 6.09×10-9 were obtained for the carbon dioxide-methane mixture. The final output of the ANN-GA via input variables can be achieved by the parameters (weights and biases) of the developed ANN. The obtained correlations were reported in Table 2. The hyperbolic tangent sigmoid transfer function (F_{hts}) is considered for hidden layers:

$$F_{hts}(x)=\frac{e^{x}-e^{-x}}{e^{x}+e^{-x}} \tag{5}$$

A comparison between the model prediction values of the thermal conductivity and the experimental data is shown in Figures 3 and 4. It is tried to prove the validation of the ANN-GA model in estimating the target data. The best fit, in which the predictions are equal to the target values, was appeared by a solid line. The figures indicate a proper coordination between the model estimated values and the experimental data. Moreover, the accuracy of the developed ANN-GA model has been studied through the testing data group (thirty percent of the data) which was not applied to the training stage.

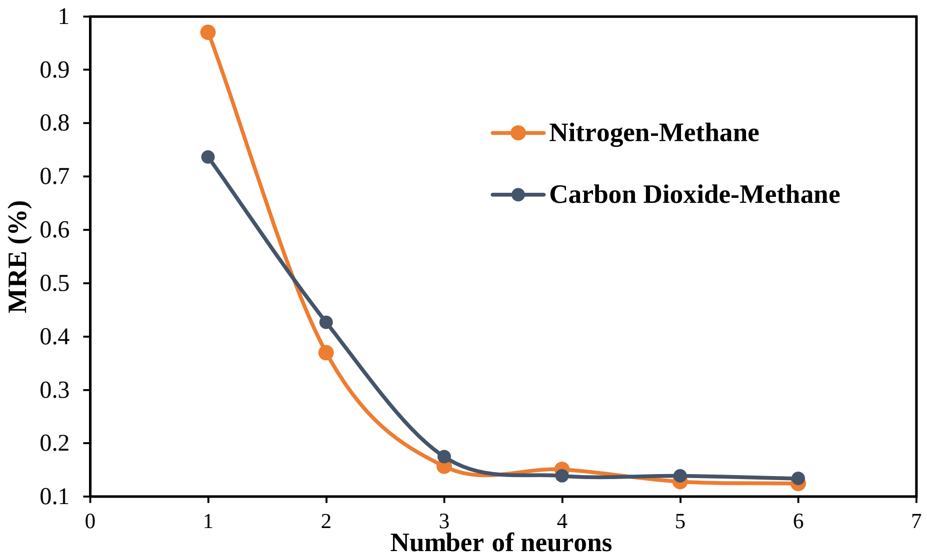


Figure 2. Performance of the ANNs with different numbers of hidden layer neurons.

Table 2
Developed correlations using ANNs.

Gas mixture	Correlation
Nitrogen-Methane	λ=0.0941-0.0104$F_{hts}\left(-0.2266x_{CH_4}+0.2548T-0.8966P-0.1157\rho+1.1059\right)$ $-0.0108F_{hts}\left(0.8636x_{CH_4}-0.4447T+0.0280P+0.3750\rho-0.7810\right)$ $+0.0844F_{hts}\left(0.2610x_{CH_4}+0.2559T-0.2166P+0.3497\rho-0.9995\right)$
Carbon Dioxide-Methane	λ=0.0623-0.0573$F_{hts}\left(-0.6033x_{CH_4}-1.6382T+0.3369P-1.5725\rho+4.3565\right)$ $-0.0307F_{hts}\left(-0.4764x_{CH_4}+1.6682T+3.7421P-5.0307\rho-3.1253\right)$ $+0.0718F_{hts}\left(0.5522x_{CH_4}+1.0274T-1.2815P+1.0948\rho-1.2048\right)$

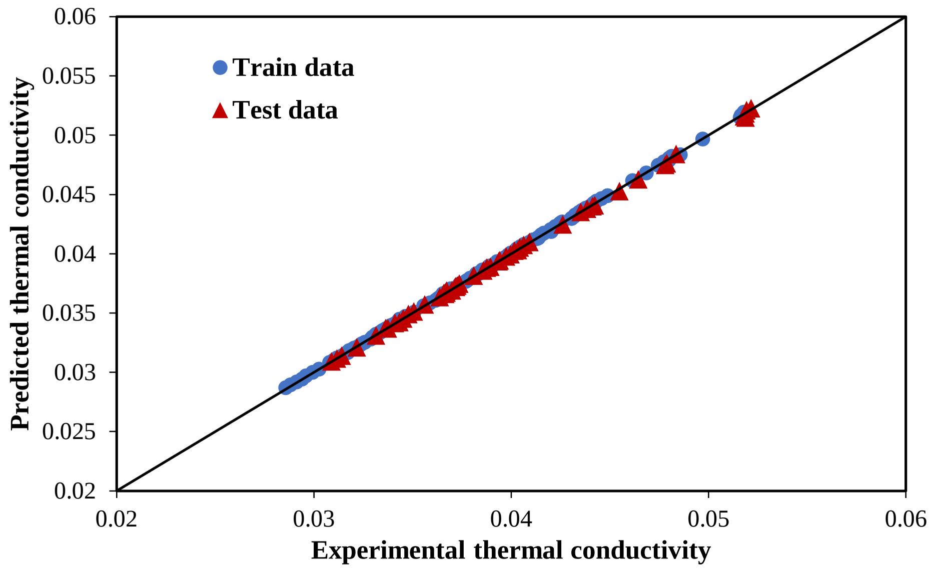


Figure 3. Predicted versus experimental data for the thermal conductivity of Nitrogen-Methane.

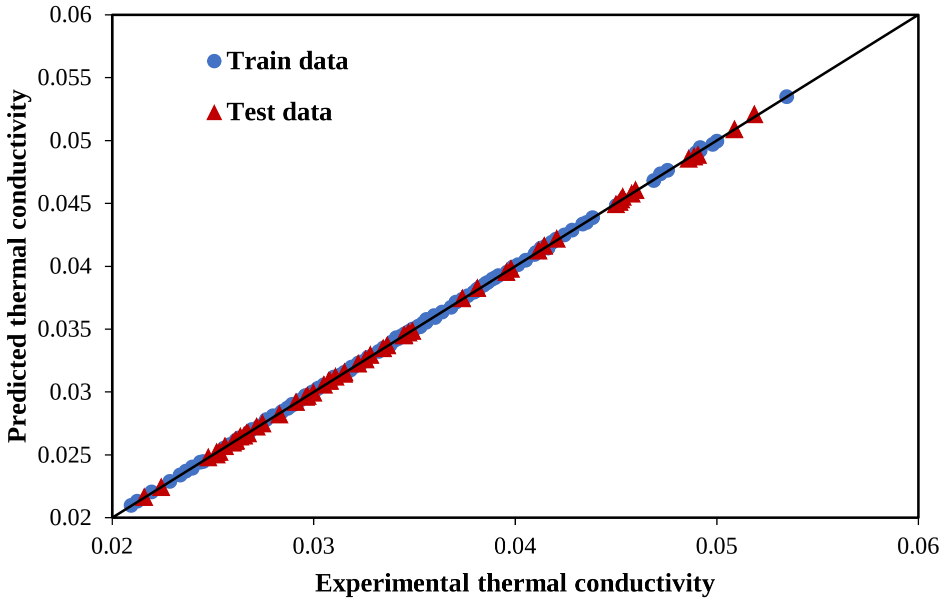


Figure 4. Predicted versus experimental data for the thermal conductivity of Carbon dioxide–Methane.

Table 3 reports the error values related to the developed ANN-GA for testing and training data. In addition, the estimation results from the investigation were compared with corresponding correlations in the literature [29, 30]. As seen in the table, the ANN–GA models have a superior performance for approximating the thermal conductivity of the investigated gas mixtures.

Table 3
Deviations of the developed ANN and literature correlations for predicting the thermal conductivity.

Gas mixture	Model	Data group	No. of data	MRE (%)	MSE
Nitrogen-Methane	ANN	Train	120	0.136	4.58×10^{-9}
		Test	51	0.206	1.44×10^{-8}
		Total	171	0.157	7.50×10^{-9}
	Vesovic and Wakeham[a] [29]			2.61	9.96×10^{-7}
	Jarrahian and Heidaryan [30]			6.312	4.24×10^{-6}
Carbon dioxide-Methane	ANN	Train	126	0.164	5.41×10^{-9}
		Test	54	0.199	7.68×10^{-9}
		Total	180	0.175	6.09×10^{-9}
	Jarrahian and Heidaryan [30]			6.678	4.87×10^{-6}

4.1. Sensitivity analysis using ANN-GA parameters

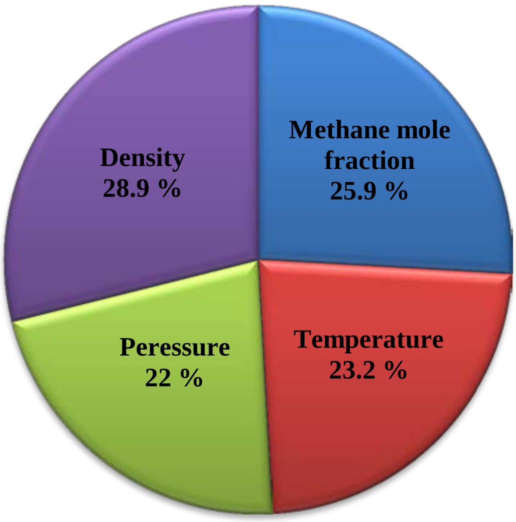
The importance of each studied effective parameter on the thermal conductivity was analyzed using the developed method [31]. The impacts (I_h) can be found using the following equation:

$$I_h=\frac{\sum_{n=1}^{n=N_j}\left(\left(\left|W_{hn}^{hj}\right|/\sum_{m=1}^{N_i}\left|W_{mn}^{ij}\right|\right)\times\left|W_{no}^{jk}\right|\right)}{\sum_{m=1}^{m=N_i}\left\{\sum_{n=1}^{n=N_j}\left(\left(\left|W_{mn}^{ij}\right|/\sum_{m=1}^{N_i}\left|W_{mn}^{ij}\right|\right)\times\left|W_{no}^{jk}\right|\right)\right\}} \tag{6}$$

where N is the number of neurons, the superscripts of i, j and k have been used to specify the input, hidden and output layers respectively, and 'm', 'n' and 'o' have been used to specify the input, hidden and output neurons respectively.

Figure 5 illustrates the percentage of the influence of each considered variable including the methane mole fraction (x_{CH4}), temperature (T), pressure (P), and density (ρ) on the thermal conductivity for two investigated systems. As shown, it is clear that all input parameters have major influences on the thermal conductivity. The gas mixture density, with the impact percentages of 28.9 and 34.9 % on the output parameter for nitrogen-methane and carbon dioxide-methane mixtures respectively, has the greatest influence.

(a)



(b)

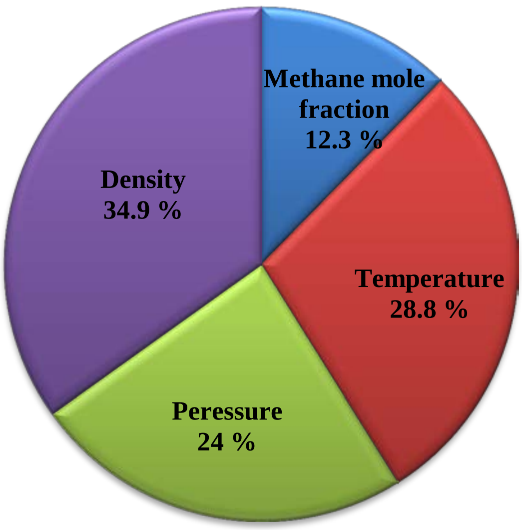


Figure 5. Importance (%) of the studied variables on the thermal conductivity for (a) Nitrogen-Methane and (b) Carbon Dioxide–Methane.

5. Conclusions

Two simple and precise correlations were developed by genetic algorithm-based neural networks to predict the thermal conductivity of nitrogen-methane and carbon dioxide-methane mixtures. Four effective parameters including the methane mole fraction, temperature, pressure, and density were considered as input variables. In the work, dividing, selecting, and normalizing were used for data pre-processing. The optimum configurations of the ANNs with three neurons in the hidden layer were obtained by the trial-and-error method. The prediction accuracy of the neural network-based correlations for the testing data indicates the ability to estimate the thermal conductivity of the investigated systems with a significantly lower deviation than that of other alternative correlations. The use of the genetic algorithm in this work guarantees the finding of optimal ANN parameters (weights and biases). The accuracy of the developed ANN models was compared with recent models presented in the literature. The results show that the ANN-GA models have a superior performance for approximating the thermal conductivity of the investigated gas mixtures. A sensitivity analysis proved that all the studied parameters affected the thermal conductivity and the effect of density was greater than that of other variables. From the study, it can be concluded that a neural network is an appropriate approach for the thermal conductivity modeling in natural gases.

Nomenclature

b_J	bias
F	transfer function
N	number of data
P	pressure [kPa].
T	temperature [K].
W_{JI}	weight
Y	model output
Greek symbols	
λ	thermal conductivity [W/m.K].
ρ	density [mol/m^3].
Subscripts	
i	input layer
j	hidden layer
k	output layer
m	input neurons
n	hidden neurons
o	output neurons
Abbreviations	
MRE	Mean relative error
MSE	Mean square error

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