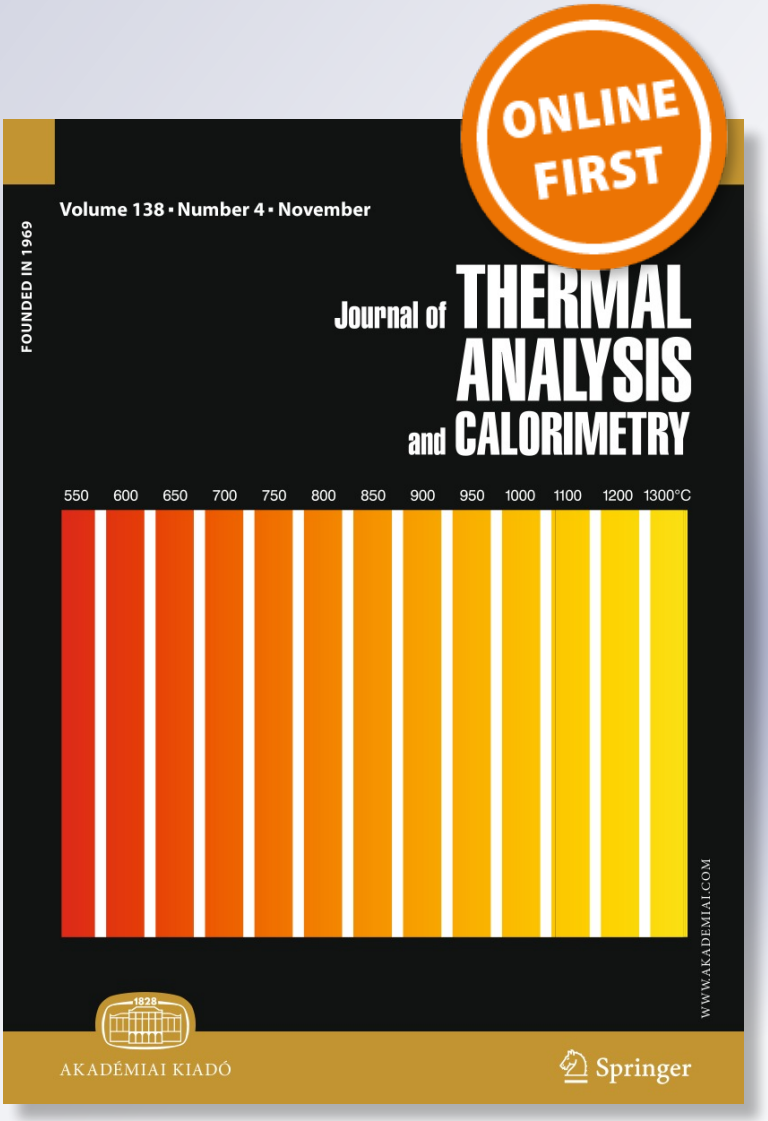
Machine learning methods for precise calculation of temperature drop during a throttling process

M. Farzaneh-Gord, H. R. Rahbari, B. Mohseni-Gharyehsafa, A. Toikka & I. Zvereva

Journal of Thermal Analysis and Calorimetry
An International Forum for Thermal Studies

ISSN 1388-6150

J Therm Anal Calorim
DOI 10.1007/s10973-019-09029-3



Springer

Journal of Thermal Analysis and Calorimetry
https://doi.org/10.1007/s10973-019-09029-3

Machine learning methods for precise calculation of temperature drop during a throttling process

M. Farzaneh-Gord[1] · H. R. Rahbari[1] · B. Mohseni-Gharyehsafa[2] · A. Toikka[3] · I. Zvereva[3]

Received: 6 July 2019 / Accepted: 5 November 2019

Abstract

It is vital for the designers of the throttling facilities to predict natural gas temperature drop along a throttling valve exactly. Generally, direct prediction of the temperature drop is not possible even by employing equations of states. In this work, artificial neural network method, specifically multilayer perceptron, is utilized to predict the physical properties of natural gas. Then, the method is employed for direct calculation of the temperature drop along a throttling process. To train, validate and test the network, a large database of natural gas fields of Iran plus some experimental data (30,000 random datasets) are gathered from the literature. In addition, according to complexity of the multilayer perceptron model, a group method of data handling approach is used to simplify the major trained network. For the first time, an equation is developed for calculating natural gas temperature drop as a function of molecular weight as well as pressure drop. The results show that the multilayer perceptron and group method of data handling methods have the error $R^2 = 0.998$ and $R^2 = 0.997$, respectively. In addition, the results indicate that both developed machine learning methods present a high accuracy in the calculations over a wide range of gas mixtures and input properties ranges.

Keywords Throttling process · Artificial neural network · Multilayer perceptron · Group method of data handling · Natural gas temperature drop · Natural gas compositions effects

List of symbols

f	Activation function
T	Temperature (K)
P	Pressure (kPa)
J	Jacobian matrix
Z	Z-factor
X	Mole fraction
v	Gas volume
R	Gas constant (J K^{-1} mol^{-1})
α	Helmholtz free energy
δ	Reduced fluid mixture
$\beta_{v,ij}, \gamma_{T,ij}, \beta_{T,ij}, \gamma_{T,ij}$	Binary mixtures parameters of GERG2008 EOS
α^0	Helmholtz free energy ideal part of gas mixture
α^0_{0i}	Ideal dimensionless Helmholtz free energy of the component i of GERG2008 EOS
$n_{ij,k}, d_{ij,k}, t_{ij,k}, \eta_{ij,k}, \varepsilon_{ij,k}, \beta_{ij,k}, \gamma_{ij,k}$	Parameters of GERG2008 EOS
α^r	Reduced Helmholtz free energy residual part
ρ	Density
τ	Inverse reduced temperature (1/K)
α^r_{or}	Generalized departure function
ω_i	Acentric factor of component i
$a, b, a_i, b_i, a_{ii}, b_{ii}, a_{ij}, b_{ij}, k_{ij}, m_i, \alpha_i$	Mixing rules parameters of cubic EOSs
n	Number of data points
R	Correlation coefficient

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s10973-019-09029-3) contains supplementary material, which is available to authorized users.

✉ M. Farzaneh-Gord
m.farzanehgord@um.ac.ir

[1] Faculty of Mechanical Engineering, Ferdowsi University of Mashhad, Mashhad, Iran

[2] Faculty of Mechanical Engineering, Shahrood University of Technology, Shahrood, Iran

[3] Department of Chemical Thermodynamics and Kinetics, Institute of Chemistry, Saint Petersburg State University, Saint Petersburg, Russia

Published online: 19 November 2019

N	Number of natural gas components, $N=21$
$P_{c,i}$	Critical pressure for component i
$T_{c,i}$	Critical temperature for component i
P_{pc}	Pseudo-critical pressure, $P_{pc}=\sum_{i=1}^{N} P_{c,i} \times X_i$
T_{pc}	Pseudo-critical temperature, $T_{pc}=\sum_{i=1}^{N} T_{c,i} \times X_i$
P_{pr}	Pseudo-reduced pressure, $P_{pr}=\frac{P}{P_{pc}}$
T_{pr}	Pseudo-reduced temperature, $T_{pr}=\frac{T}{T_{pc}}$
W	Weights matrix

Subscripts

c	Critical point
r	Reduced

Abbreviations

AAPD	Average absolute percent deviation
ANN	Artificial neural network
EOS	Equations of state
GMDH	Group method of data handling
HFE	Helmholtz free energy
JT	Joule–Thomson
NG	Natural gas
MLP	Multilayer perceptron

Introduction

Natural gas throttling is a common process in natural gas industry in which the gas stream must be suddenly expanded from the high pressure to lower pressure. This is mainly an isenthalpic process and causes a significant change in the physical properties of the mixture, especially its temperature falls sharply [1]. In a natural gas pressure drop station, for instance, the temperature of the natural gas after the expansion process is a key parameter such that it should not approach the hydrate forming zone [2] Therefore, it is essential that the process be such designed that the natural gas flow does not fall into the trap of hydrate formation. For a proper design and dimensioning of the throttling process, precise information about the behavior of the gas flow through the expansion process is required. The determination of the thermodynamic properties of natural gas, however, is challenging as it usually comes in the form of heavy mixtures. Apart from the metering instruments that may be used for the direct measurement of only some of the physical properties, such as temperature, pressure and speed of sound, the further properties of natural gas can only be calculated by the equation of states (EOSs) or other theoretical methods [3].

In fact, the EOSs define the thermodynamic properties of the natural gas mixtures as functions of their measurable properties. Of the several developed EOSs, as the only method of determining the physical properties of the natural gas mixtures so far, GERG2008 [4] and AGA8 [5] are two of the most commonly used and referenced ones. The main and common disadvantage of these equations, however, is that they only accept the temperature, pressure and compositions as the input for the direct calculation of the other thermodynamic properties [6]. Although these equations may still be employed with different input data, an iterative solution would be required in this case, which is time-consuming and even has inaccuracies sometimes. Therefore, it is not the cleverest measure to use such EOSs for designing the throttling processes for which the enthalpy, the pressure and the compositions are the primary, secondary and side effective parameters.

There is an extensive literature focusing on finding an alternative method for the calculation/estimation of one or some thermodynamic properties of natural gas mixtures in various conditions. For example, in the two studies, the correlations are presented for calculating the natural gas density [7, 8].

In one study, the alternating conditional expectations algorithm is proposed to estimate the viscosity and density of natural gas mixtures [9]. Farzaneh-Gord and Rahbari [10] developed the novel correlations for calculating thermodynamic properties of natural gas. In their study, the average absolute percent deviation (AAPD) for compressibility factor calculations was 0.674%, for density was 2.55% and for Joule–Thomson coefficient was 4.16% [11]. In recent studies, Farzaneh-Gord et al. [12] developed two novel correlations for calculating the density and the molecular weight of natural gas mixtures as functions of three directly measurable properties of temperature, pressure and Joule–Thomson coefficient, and temperature, pressure and sound speed, respectively. Many more studies could be addressed here that have conducted research in this topic, but to the extent of the authors' knowledge, there is no study that specifically investigates a throttling process design condition.

Artificial neural network (ANN) methods or connectionist systems are computing systems vaguely inspired by the biological neural networks that constitute brains. The neural network itself is not an algorithm, but rather a framework for many different machine learning algorithms to work together and process complex data inputs. Such systems "learn" to perform tasks by considering examples, generally without being programmed with any task-specific rules. An ANN is based on a collection of connected units or nodes called

artificial neurons, which loosely model the neurons in a biological brain. Each connection, like the synapses in a biological brain, can transmit a signal from one artificial neuron to another. An artificial neuron that receives a signal can process it and then signal additional artificial neurons connected to it. Typically, artificial neurons are aggregated into layers. Different layers may perform different kinds of transformations on their inputs. Signals travel from the first layer (the input layer) to the last layer (the output layer), possibly after traversing the layers multiple times [13]. The ANN has widely been used in many scientific areas due to the high accuracy, high solution speed and less complication of this method compared to the traditional methods. For example, Gill et al. [14] used artificial intelligence method to predict the destruction of exergy in components of a LPG refrigeration system. Their work shows that the proposed method could be predicted the destruction of exergy in the components of refrigeration system quickly and with high accuracy. Ramezanizadeh et al. [15] presented a review of application of intelligence methods, including ANNs to predict thermal conductivity of nanofluids. The results of their work show that the ANNs have higher precision than other intelligence methods. Ahmadpour et al. [16] developed an optimization method based on ANNs to optimize the natural gas condensate hydrodesulfurization unit. Their work shows that the proposed method could optimize the objective function very fast with high accuracy.

Intelligence methods such as ANN techniques are employed and widely used for analyzing heat and mass transfer. For example, Ahmadi et al. [17] employed the different intelligent methods to predict thermal conductivity and dynamic viscosity of Fe_2O_3/water nanofluid. The results of their study show that the RBF neural network algorithm based on genetic algorithm (GA-RBF algorithm) has the highest R^2 values for predicting the physical properties of Fe_2O_3/water nanofluid. Baghban et al. [18] estimated the convective heat transfer coefficient of nanofluids in circular cross-sectional channels. In their study, seven different models were applied and compared with each other. The results of their work indicate that these proposed models are very useful for prediction of convective heat transfer coefficient of nanofluid. Maddah et al. [19] predicted the viscosity of multiwall carbon nanotube by applying the ANN and self-organizing map methods. The results of their study show that the ANN method can predict the viscosity with acceptable accuracy. Ramezanizadeh et al. [20] presented a precise model to predict the dynamic viscosity of Al_2O_3/water nanofluid. In their study, four ANN models were employed to estimate the viscosity of Al_2O_3/water nanofluid. In another study, Ahmadi et al. [21] employed two intelligent methods to predict the thermal conductivity ratio of Al_2O_3/EG nanofluid. The results of their work show that the proposed methods could estimate the thermal conductivity of the nanofluid with applicable accuracy. Also, in a recent study, Bagheri et al. [22] used ANN method to optimize free convection of hybrid nanofluids in a c-shaped chamber. The results of their work show that the ANN using the PSO algorithm can optimize the Nusselt number with high accuracy.

However, ANN is not used frequently in the natural gas industries simulation. The pioneers of employing the ANN approaches for the property estimation of gases are Moghadassi et al. [23]. Their study was a simple model to estimate the temperature, pressure and specific volume of pure gases, although most studies in this area were related to natural gas compressibility factor calculation. For example, in a study, the more complicated model developed to calculate natural gas compressibility factor [24]. Al-Anzari et al. [25] developed the ANN method for estimating the compressibility factor of sour natural gas mixtures and reported an average absolute error just below 1%. In a similar work, Sanjari and Lay [26] developed an ANN model to calculate the natural gas compressibility factor using large training and testing database comprising a total of 5500 experimental data. Some researchers compared the ANN method with other machine learning methods such as the fuzzy inference system (FIS) and the adaptive neuro-fuzzy inference system (ANFIS) in the case of predicting the compressibility factor of a natural gas mixture [27]. Comparing the obtained results with the results given by the EOSs, they found their trained ANN model more accurate than all the other approaches. Finally, as one of the latest works in this research field, Azizi et al. [28] estimated the natural gas compressibility factor by training an ANN model using Standing and Katz diagram, though their effort did not result in satisfactory findings.

In this work, the multilayer perceptron (MLP) method, as one of the machine learning methods, is employed to predict temperature drop during a throttling process. For such a process, the known properties are the enthalpy, the pressure and the compositions of the natural gas mixture. Therefore, the MLP model is developed based on these three physical properties as the input data. The output information of the model includes the temperature and the compressibility factor. It could be shown that the MLP method is very fast with higher accuracy compared to EOSs. A randomly made database consisting of properties such as natural gas compositions, temperatures and pressures was utilized to train the desired MLP model. In addition, for the first time an equation has been developed for calculating temperature drop due to pressure drop as a function of molecular weight. For validating and testing the trained model, a huge database including the physical properties of four natural gas fields of Iran, namely Pars, Khangiran, Sarjeh and Sarkhoon, as well as some experimental data gathered from the literature are used. Also, according to the complexity of the major MLP model which contains 23 inputs, data consist of 21 mole fractions of the natural gas, pressure and temperature,

and a group method of data handling (GMDH) neural network approach is used to tackle this issue. In the GMDH approach, for obtaining temperature drop through throttling processes just molecular weight of the natural gas, inlet and outlet pressure and inlet temperature are required.

Problem discussion

Throttling valves usually called Joule–Thomson (JT) valves are widely employed in natural gas industries for natural gas pressure reduction. Figure 1 shows two-sample utilization of these valves. For separating heavier parts of natural gas stream, a sample configuration shown in Fig. 1a is utilized [29]. The same process is utilized for recovering ethane from natural gas stream in the natural gas refineries. Natural gas passes through a heat exchanger for pre-cooling before entering the JT valve. As natural gas exits the valve with lower pressure and temperature, it enters a flash separator that separates the liquid phase from the gas phase. The natural gas temperature has the most important influence on the separation efficiency of the system. The designers should know how temperature drop is related to pressure drop and natural gas compositions. A typical natural gas pressure drop station is shown in Fig. 1b as the other example [30]. In these stations, it is very important to know the properties of the gas after the JT valve and the temperature drop along the expansion process is the most important factor. Designers should be able to design and size the required heaters in order to prevent the gas to fall down behind hydrate forming temperature.

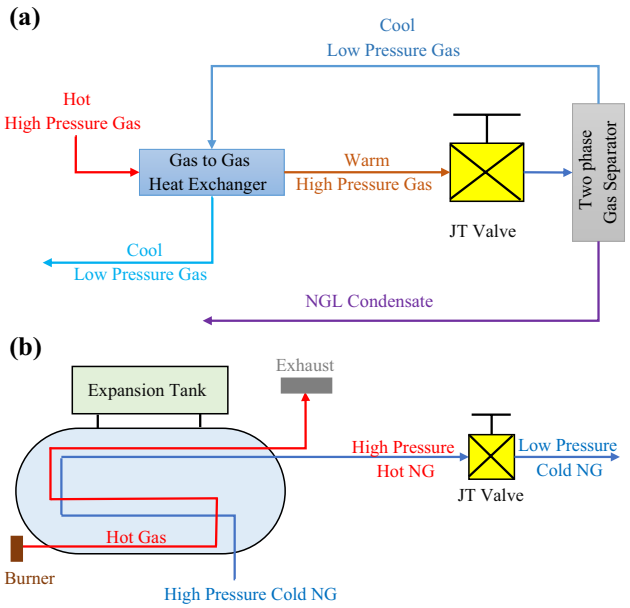


Fig. 1 Typical utilization of throttling valve (JT valve) in natural gas industries. **a** Recovering heavier hydrocarbon, **b** a pressure drop station

The above examples clearly indicate the importance of knowing the exact amount of temperature drop due to pressure drop in a JT valve. The usual approach for computing the temperature drop in a JT valve is to employee an EOS with an iterative method. As the process across a JT valve is an isenthalpic process, the temperature after the valve could be computed by varying outlet temperature until the inlet and outlet enthalpies get very close.

In this study, a novel approach has been employed to compute the temperature drop and consequently outlet temperature of an expansion process by utilizing machine learning method. The MLP and the GMDH are two sub-models of ANN that have been used in this study as machine learning method. For designing the valve and the ancillary facilities coming with it, a gas flow is supposed to come into the expansion device with P1 and T1. Using the proposed two ANNs, the designer could calculate the outlet temperature for the natural gas mixture directly.

Methodology

To develop the proposed ANN approach for calculating the temperature drop across an expansion process, firstly, a database of pressure and temperature before and after a JT valve for various natural gas compositions should be created. The required data could come from experimental data, theoretical data or both. In this study, the GERG2008 EOS as the most recent and authentic EOS for calculating natural gas thermodynamic properties has been employed. In this section, firstly, the GERG2008 EOS has been introduced. Then, the MLP method and the GMDH method as two machine learning methods have been discussed. These two ANNs are the alternative approaches for predicting the physical properties of natural gas mixture through throttling processes.

GERG2008 EOS

The GERG2008 EOS basically combines the well-developed pure gas EOSs into a single EOS for the natural gas mixtures. This EOS is explicit in the Helmholtz free energy (HFE). The HFE of a fluid mixture is a function of its density, temperature and compositions as below [4]:

$$\alpha\left(\rho, T, \bar{X}\right) = \alpha^{0}\left(\rho, T, \bar{X}\right) + \alpha^{\mathrm{r}}\left(\rho, T, \bar{X}\right), \tag{1}$$

where ρ, T and $\bar{X}$ are the density, temperature and the molar content of the compositions in the mixture. The function α° represents the properties of ideal gas mixtures at the given values of ρ, T and $\bar{X}$, while α^{r} takes into account the residual

mixture behavior. These two parameters are defined as below [4]:

$$\alpha^0\left(\rho,T,\bar{X}\right)=\sum_{i=1}^{N}X_{\mathrm{i}}\left[\alpha_{0\mathrm{i}}^0(\rho,T)+\mathrm{Ln}\left(X_{\mathrm{i}}\right)\right] \tag{2}$$

$$\alpha^{\mathrm{r}}\left(\delta,\tau,\bar{X}\right)=\alpha_0^{\mathrm{r}}\left(\delta,\tau,\bar{X}\right)+\Delta\alpha^{\mathrm{r}}\left(\delta,\tau,\bar{X}\right), \tag{3}$$

where in the former, $\sum X_{\mathrm{i}}\mathrm{Ln}\left(X_{\mathrm{i}}\right)$ accounts for the entropy of ming, and $\alpha_{0\mathrm{i}}^0(\rho,T)$ is the dimensionless HFE of component i in the ideal gas state, and in the latter, $\alpha_{\mathrm{or}}^{\mathrm{r}}$ is the residual part of the reduced HFE of component i, and $\Delta\alpha^{\mathrm{r}}$ is the specific departure function developed for the respective binary mixtures.

In Eq. 3, δ and τ are, respectively, the reduced mixture density and the inverse reduced mixture temperature given by [4]:

$$\delta=\frac{\rho}{\rho_{\mathrm{r}}\left(\bar{X}\right)} \tag{4}$$

$$\tau=\frac{T_{\mathrm{r}}\left(\bar{X}\right)}{T} \tag{5}$$

in which [4]:

$$\frac{1}{\rho_{\mathrm{r}}\left(\bar{X}\right)}=\sum_{i=1}^{N}\sum_{j=1}^{N}X_{\mathrm{i}}X_{\mathrm{j}}\beta_{\mathrm{v,ij}}\gamma_{\mathrm{v,ij}}\frac{X_{\mathrm{i}}+X_{\mathrm{j}}}{\beta_{\mathrm{v,ij}}^2x_{\mathrm{i}}+x_{\mathrm{j}}}\left[\frac{1}{8}\right]\left(\frac{1}{{}^1/_3}+\frac{1}{{}^1/_3}\right)^3 \tag{6}$$

$$T_{\mathrm{r}}\left(\bar{X}\right)=\sum_{i=1}^{N}\sum_{j=1}^{N}X_{\mathrm{i}}X_{\mathrm{j}}\beta_{\mathrm{T,ij}}\gamma_{\mathrm{T,ij}}\frac{X_{\mathrm{i}}+X_{\mathrm{j}}}{\beta_{\mathrm{T,ij}}^2X_{\mathrm{i}}+X_{\mathrm{i}}}\left(T_{\mathrm{c,i}}\cdot T_{\mathrm{c,j}}\right)^{0.5}. \tag{7}$$

Here δ and τ are developed based on quadratic mixing rules. $\beta_{\mathrm{v,ij}}$, $\gamma_{\mathrm{T,ij}}$, $\beta_{\mathrm{T,ij}}$ and $\gamma_{\mathrm{T,ij}}$ are binary mixture parameters, and their values along with the value of the critical parameters $\rho_{\mathrm{c,i}}$ and $T_{\mathrm{c,i}}$ of the pure components could be found in ISO 20765-2 [31].

Due to the abundance of the references on the GERG2008, no further discussion on this matter is presented. The only remaining noteworthy point is that as the actual input values in natural gas industries are pressure, temperature and natural gas components, an iterative method is required to find the pressure value first, and then any other physical properties. The validity of GERG2008 EOS is proved for the normal ranges of 90 K ≤ T ≤ 450 K and P ≤ 35,000 kPa, while this range can even be extended to 60 K ≤ T ≤ 700 K and P ≤ 70,000 kPa.

In spite of many advantages that GERG2008 offers, there are some drawbacks that restrict its applications in some situations. Some of these deficiencies are:

- The inflexibility of the EOS in the input data as it only accepts pressure, temperature and compositions
- Difficult implementation and the high possibility mistakes during the coding process of the EOS
- The occasional inaccurate response of the EOS in the conditions that the thermodynamic behavior of the mixture does not follow a regular manner.

MLP method

The ANN is one of the powerful methods for function approximation and simulation, whose procedure is inspired by behavior of biological cell nerves. The main aim of artificial neural networks is structuring a mathematical relationship between an input and output dataset. The most common type of ANN is the MLP method. The MLP generally consists of three layers, named as input layer whose neurons are the independent variables of problem, hidden layer whose neurons form a relationship between independent and dependent variables and output layer whose neurons contain the dependent variables. The MLP neural network has many parameters and components. The three main components of this ANN are data collected for the training and weights, the biases and the algorithms for training networks.

Data typically collected for training neural networks are divided into three categories, namely training data, validation data and test data. Training data are directly engaged in the training process, and validation dataset is used to show the deviation during training networks and is not directly involved in training algorithm and altering the weights and biases. The testing dataset is used to check performance of the MLP for data that did not participate in the training process. Weights and biases are adaptive coefficients that determine the effectiveness of Inputs. These coefficients are first determined as random and then optimized by a training algorithm. Figure 2 shows a simple network that consists of an input layer, one hidden layer (with two neurons) and an output layer. The method for obtaining the desired output is given in Eqs. (8)–(10):

$$\mathrm{neuron}_1^1=\begin{cases}\mathrm{net}_1^1=\sum_{i=1}^{n_0}W_{1\mathrm{i}}^1\times X_0\\ o_1^1=f\left(\mathrm{net}_1^1\right)\end{cases} \tag{8}$$

$$\mathrm{neuron}_2^1=\begin{cases}\mathrm{net}_2^1=\sum_{i=1}^{n_0}W_{2\mathrm{i}}^1\times X_{\mathrm{i}}\\ o_2^1=f\left(\mathrm{net}_2^1\right)\\ V\triangleq\left[V_0,o_1^1,o_2^1,\ldots\right]^{\mathrm{T}}\end{cases} \tag{9}$$

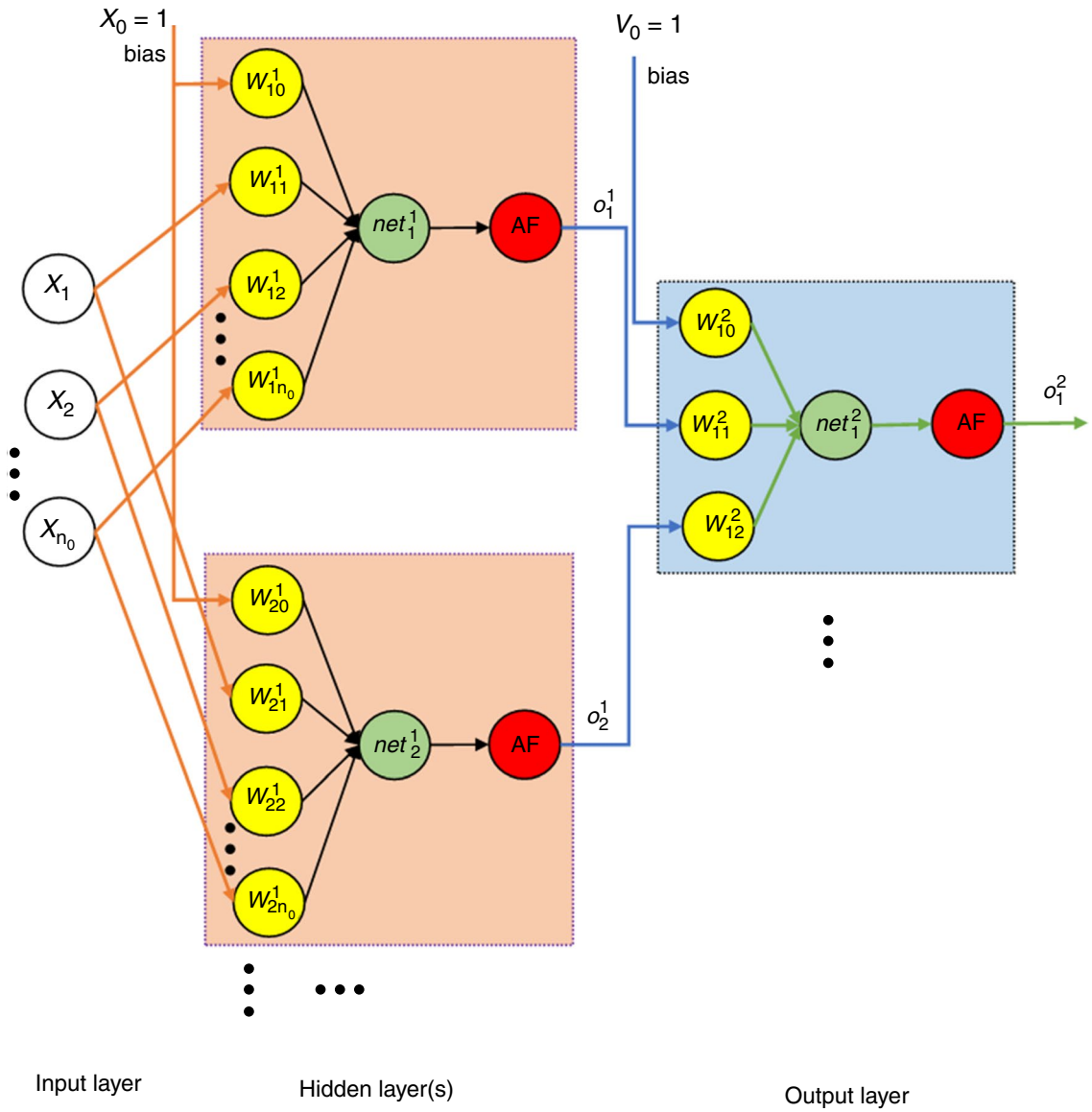


Fig. 2 Sample MLP method as an artificial neural network

$$\text{neuron}_1^2 = \begin{cases} \text{net}_1^2 = \sum_{i=0}^{n_0} W_{1i}^2 \times V_i \\ o_1^2 = f\left(\text{net}_1^2\right) \end{cases}. \tag{10}$$

In ANN, the activation function of a node defines the output of that node, or "neuron," given an input or set of inputs. It should be noted that the activation functions used in MLP neural networks are tangential hyperbolic (tansig) function. This function has been introduced in Eq. (11). The linear function is usually used in hidden layers, and the activation function for the output layer is usually linear function. The linear function has been introduced in Eq. (12) [32]:

$$f(a) = \tanh(a) = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}; [-1, 1] \tag{11}$$

$$f(a) = a; (-\infty, \infty). \tag{12}$$

According to the above paragraph, the network must be trained by a training algorithm. There are many algorithms for training. One of the accurate algorithms for training neural networks is backpropagation learning algorithm. There are several backpropagation training methodologies, but the most powerful methodology is Levenberg–Marquardt. Equation (13) shows the Levenberg–Marquardt formula for obtaining optimum weights and biases in neural networks [32]:

$$W^{(k+1)} = W^{(k)} - \left(\left[J^{T} \cdot J + \mu I\right]^{-1}\right) \cdot \left(J^{T} \cdot e\right), \quad (13)$$

where J is the Jacobian matrix, e is the difference between network output and its target and I is a diagonal matrix that its entries are the main diagonal of $J^{T} \cdot J$.

The input information of this current model is the pressure, the enthalpy and the molar fractions of the natural gas compositions (21 components in total), as the three key properties are required to analyze a gas throttling process. The outputs of the model include several physical properties of the mixture including the compressibility factor and the temperature.

Table 1 gives a detailed report of the number of neurons in each layer, the number of layers, the input data, the proportion of database used for training, validating, testing, etc. In Table 1, R is the correlation coefficient for each input data given by [32]:

$$R = \frac{n\left(\sum_{i=1}^{n} a_i t_i\right) - \left(\sum_{i=1}^{n} a_i\right)\left(\sum_{i=1}^{n} t_i\right)}{\sqrt{n\sum_{i=1}^{n} a_i^2 - \left(\sum_{i=1}^{n} a_i\right)^2}\sqrt{n\sum_{i=1}^{n} t_i^2 - \left(\sum_{i=1}^{n} t_i\right)^2}}. \quad (14)$$

In Eq. (14), n is the total number of the training data, t_i is the target value and a_i is the network output value.

Figure 3 shows the algorithm for calculating outlet temperature using the method presented in this section. The natural gas compositions, inlet pressure and temperature are supplied for GERG2008 EOS. The EOS calculates the inlet enthalpy and transfers it along with the compositions as input for the MLP method. Based on these inputs ($h_2 = h_1$, P_2 and X_i), the MLP method calculates the outlet temperature.

Table 1 Characteristics of the developed neural network

Parameter	Value/comment
Number of input layer neurons	23
Number of hidden layers	2
Number of neurons in each hidden layer	22
Hidden layers transfer function	Tansig
Output layers transfer function	Purelin
Number of total data for this study in each ANN complex	29,871
Percentage of train data	70%
Percentage of validation data	15%
Percentage of test data	15%
R for output [T]	0.99999
R for output [Z]	0.99999
Best validation performance at Epoch	600

GMDH method

The GMDH is applied in a great variety of areas for deep learning and knowledge discovery, forecasting and data mining, optimization and pattern recognition. Inductive GMDH algorithms give possibility to find automatically interrelations in data, to select an optimal structure of model or network and to increase the accuracy of existing algorithms. This original self-organizing approach is different from deductive methods used for modeling. It has an inductive nature. It finds the best solution by sorting-out of possible variants. Criterion characteristic by sorting of different solutions of GMDH networks aims to minimize the influence of the author on the results of modeling. Computer itself finds the structure of the optimal model or laws that act in a system. The GMDH is a set of several algorithms for different problems solution. It consists of parametric, cauterization, analogs complexing, binarization and probability algorithms. This inductive approach is based on sorting-out of gradually complicated models and selection of the optimal solution by minimum of external criterion characteristic. Not only polynomials but also nonlinear, probabilistic functions or cauterizations are used as basic models [33].

Given the heaviness of the neural network due to the complexity of the subject under discussion, the temperature drop in the JT valve has been calculated using the GMDH method. In the MLP method, the enthalpy is the main input of neural network, but in the GMDH method, the inputs of this model are molecular weight, initial pressure, secondary pressure and initial temperature. To train the GMDH neural network, 4000 randomized data that are generated by the main ANN-LMA neural network have been used.

The main equation for calculating the outlet temperature of JT valve base on the GMDH method is presented in Eq. (15):

$$T_2 = A_{211} + MW \times A_{212} + MW^2 \times A_{213} + F_{39} \times A_{214}. \quad (15)$$

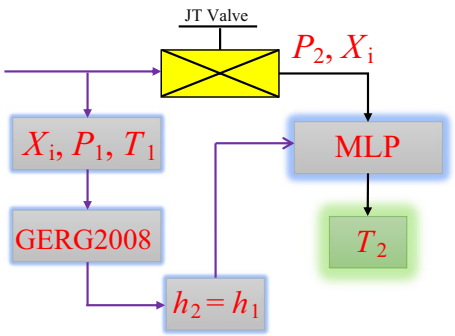


Fig. 3 MLP structure to simulated JT valve

The parameters in Eq. (15) have been calculated with equations F1–F39. These equations and the coefficients of Eq. (15) are presented as Supplementary Data.

Figure 4 shows the algorithm for calculating the outlet temperature using the GMDH method. The natural gas compositions, inlet pressure and temperature and outlet pressure are supplied as input for the method. Based on these inputs, the method calculates the outlet temperature.

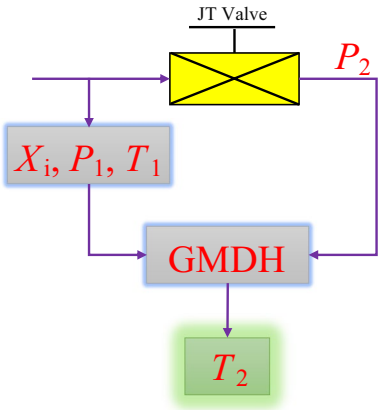


Fig. 4 GMDH structure to find the outlet temperature of a JT valve

Validating methods (GMDH and MLP)

In this section, the proposed methods have been validated by comparing the calculated results with the experimental data. The temperature drop (i.e., outlet temperature) from JT valve has been calculated for two cases. The pure methane (CH_4) [34] and the combination of 89% methane and 11% ethane ($0.89CH_4+0.11C_2H_6$) [35] have been selected for validation processes. The temperature drop has been calculated with the MLP method and the GMDH method for a few samples. According to Fig. 5, for the pure methane, the temperature drop that is calculated with the MLP is the more matching with experimental data. For the ($0.89CH_4+0.11C_2H_6$), both the MLP and the GMDH methods have calculated the temperature drop with the same precision compared with the experimental data. The validation results show that the proposed methods have calculated the temperature drop in JT valve with an acceptable accuracy.

Results and discussion

In this section, the temperature drop for various natural gases during an expansion process through a JT valve is presented and discussed. The four important natural gases from Iran's fields (see Table 2) and the pure methane have been selected to calculate the temperature drop in the JT valve by utilizing the MLP and GMDH methods. The calculations have been carried out for six different initial temperatures including 275, 300, 325, 350, 375 and 400 K. In addition, the inlet

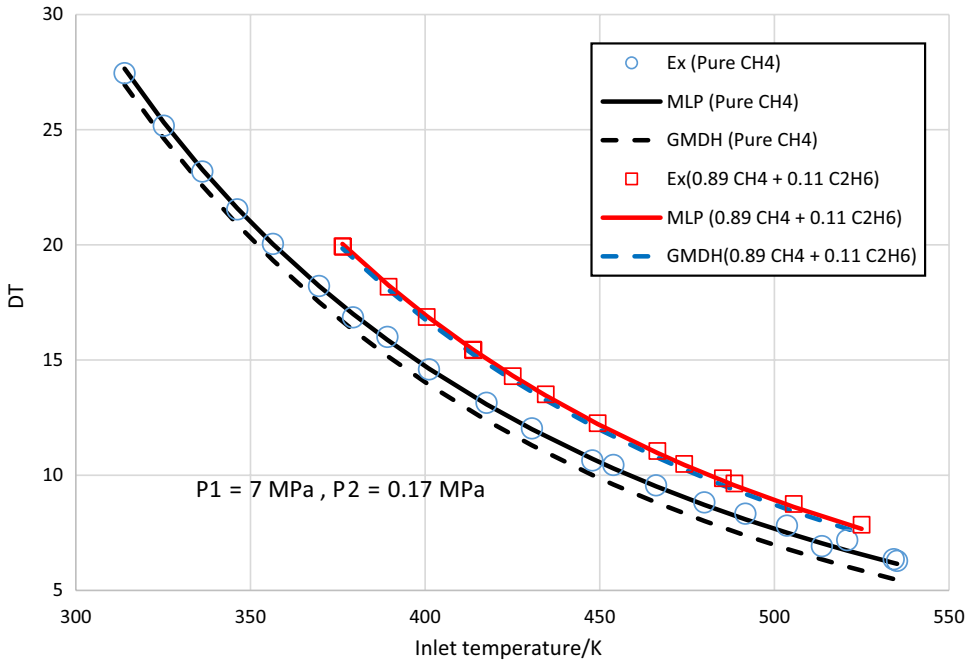


Fig. 5 Validation of temperature drop from a JT valve for pure methane (CH4) and the combination of 89% methane and 11% ethane (0.89CH4 + 0.11C2H6)

JT valve pressure has been considered between 1500 and 10,000 kPa. Furthermore, the JT valve outlet pressure has been kept constant at 600 or 900 kPa.

Figures 6 and 7 show variations of temperature drop in terms of pressure for six constant initial temperatures including 275, 300, 325, 350, 375 and 400 K for Sarkhon natural gas. Results have been calculated for output pressure of 600 kPa (Fig. 6) and 900 kPa (Fig. 7). For both pressure cases, the MLP method has been utilized for JT valve simulation. Table 3 shows the average Joule–Thomson coefficient for various inlet temperatures for Sarkhon natural gas and two outlet pressures (600 and 900 kPa). In addition, for each constant temperature line, a linear trend formula has been presented. There is a linear relationship between temperature drop and pressure drop, which is as follows:

$$DT = C_1 \times DP + C_2. \tag{16}$$

According to Figs. 6, 7 and Table 3, the coefficient C1 in Eq. (16) is very close to the average Joule–Thomson coefficient so that when the initial temperature increased, the value of C1 is closer to the average Joule–Thomson coefficient. Figures 6 and 7 show that, as expected, the temperature drop increases with increasing initial pressure at each inlet temperature and constant output pressure. It could be inferred from Figs. 6 and 7 that at low initial pressures, the temperature drop is almost the same. The temperature drop has been raised by increasing the initial temperature at each inlet and output pressure.

Figure 8 shows the temperature drop across a JT valve for pure methane and six inlet temperatures including 275, 300, 325, 350, 375 and 400 K and two outlet temperatures

Table 2 Compositions of the natural gas from important Iran's fields [36]

	Pars (NG1)	Sarjeh (NG2)	Sarkhon (NG3)	Khangiran (NG4)
Methane	0.87	0.868	0.8809	0.98548
Nitrogen	0.031	0.0205	0.0575	0.005
Carbon dioxide	0.0171	0.0011	0.0053	0
Ethane	0.054	0.0582	0.0342	0.00647
Propane	0.017	0.0303	0.0127	0.00069
Isobutane	0.003	0.0045	0.0029	0.00018
n-Butane	0.0045	0.0096	0.0037	0.00039
Isopentane	0.0013	0.0025	0.0012	0.00018
n-Pentane	0.0011	0.0027	0.0007	0.00021
n-Hexane	0.0007	0.0026	0.0009	0.0014
n-Heptane	0.0003	0	0	0
MW	18.65	19.05	18.16	16.35
$T_{cr}[K] = \sum x_i T_{ci}$	202.48	206.9916	195.9994	191.83
$P_{cr}[kPa] = \sum x_i P_{ci}$	4606.9	4560.2	4539.9	4591.4

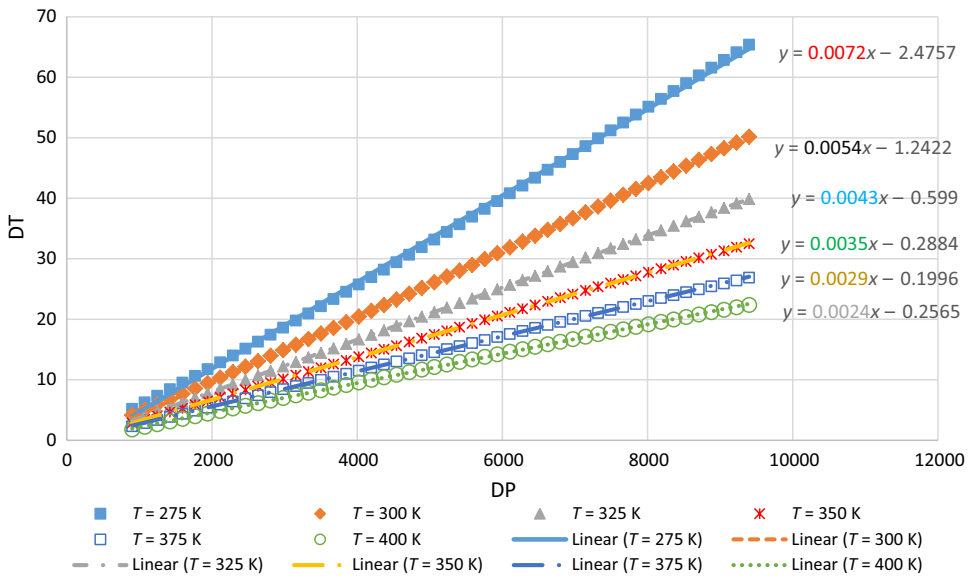


Fig. 6 Temperature drop across a JT valve for Sarkhon NG for various inlet temperatures (output pressure is kept constant at 600 kPa)

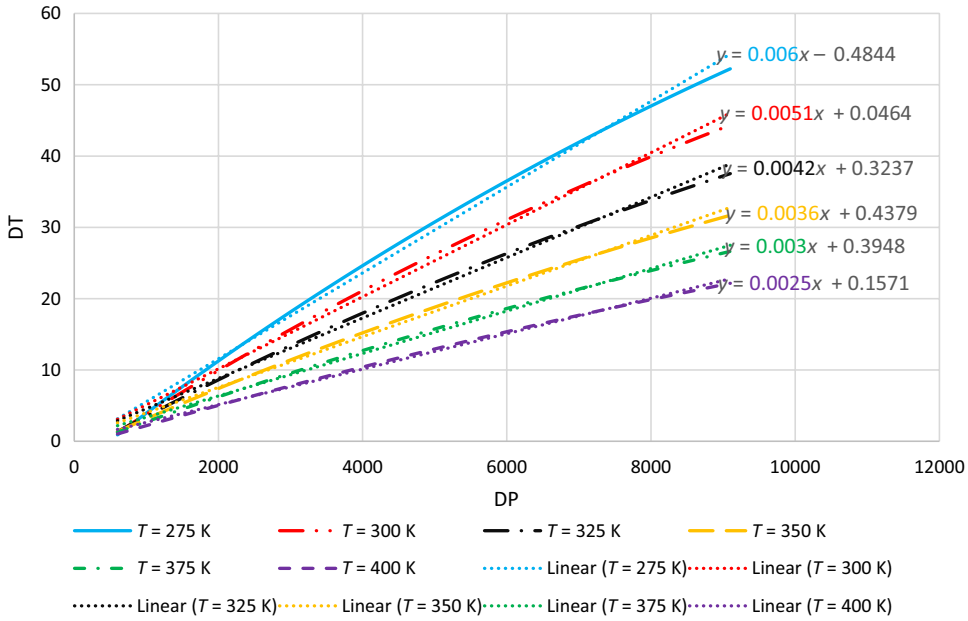


Fig. 7 Temperature drop across a JT valve for Sarkhon NG for various inlet temperatures (output pressure is kept constant at 900 kPa)

Table 3 Average Joule–Thomson coefficient for various inlet temperatures for Sarkhon gas compositions and two outlet pressures (600 and 900 kPa)

Initial temperature	275	300	325	350	375	400
Output pressure = 600 kPa						
Average Joule–Thomson coefficient	0.005248	0.004376	0.003665	0.003087	0.002614	0.002224
Output pressure = 900 kPa						
Average Joule–Thomson coefficient	0.004905	0.004095	0.003436	0.002898	0.002456	0.00209

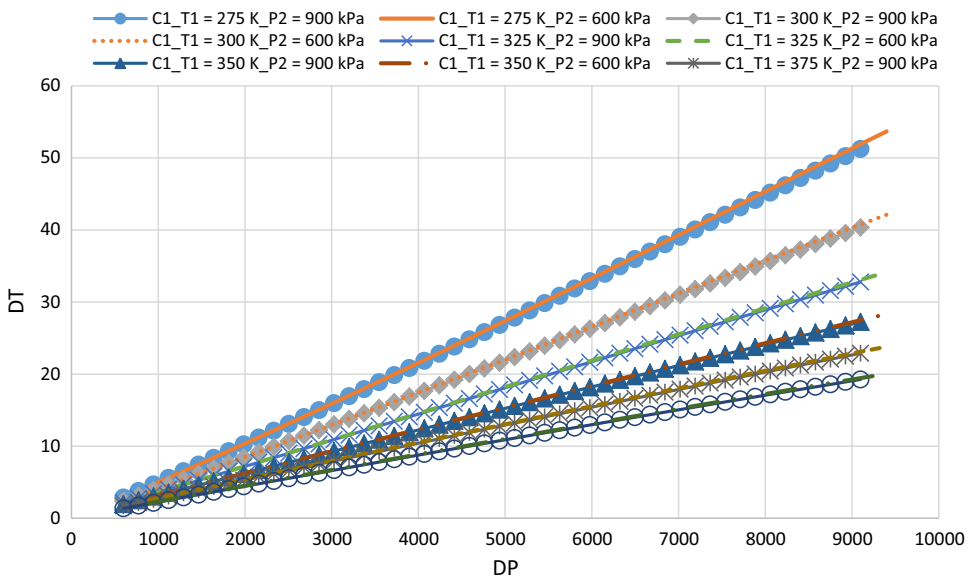


Fig. 8 Temperature drop across a JT valve for pure methane, various inlet temperatures and two outlet pressures

600 kPa and 900 kPa. According to Fig. 8, the secondary pressure that natural gas seeks to reach does not have much effect on its temperature drop. The results show that, at low initial pressures, the temperature drop is the same. In addition, the lower secondary pressure of natural gas caused the higher temperature drop in the JT valve.

Figures 9 and 10 show the temperature drop in terms of pressure slump for two fixed output pressures of 600 kPa

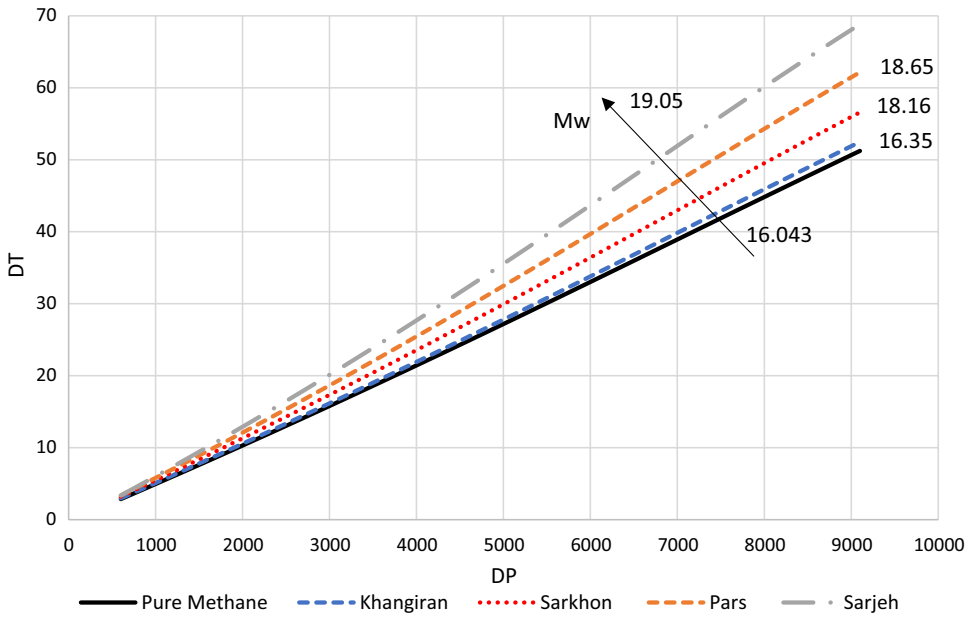


Fig. 9 Amount of temperature drop in a JT valve for various natural gases (inlet temperature = 275 K, outlet pressure = 600 kPa)

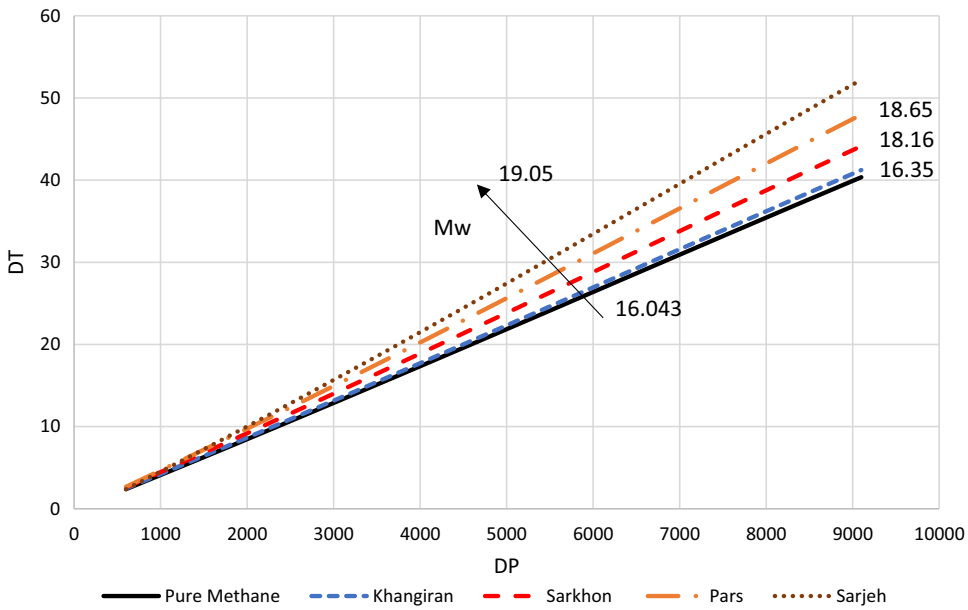


Fig. 10 Amount of temperature drop in a JT valve for various natural gases (inlet temperature = 300 K, outlet pressure = 900 kPa)

(Fig. 9) and 900 kPa (Fig. 10) at six inlet temperatures for various natural gases. It could be concluded from Figs. 9 and 10 that, unlike inlet temperature, the JT valve output pressure has small effect on the temperature drop. According to Figs. 9 and 10, the output pressure has a slight effect on the temperature drop. It could be understood from Figs. 9 and 10 that various natural gases have the same temperature drop at lower initial pressures. In addition, it could be realized that the temperature drop is directly related to the molecular weight which means that for the higher molecular weight of the natural gas, the temperature drop for the same conditions is greater.

Figure 11 shows the amount of temperature drop in JT valve for Sarkhon natural gas. In this case, the output pressure is 900 kPa. The pressure drop has been calculated by utilizing the GMDH method. The GMDH method generates the error $R^2 = 0.997$ for the temperature drop calculation. In the GMDH method, the temperature drop has been calculated with an acceptable accuracy. Using the GMDH

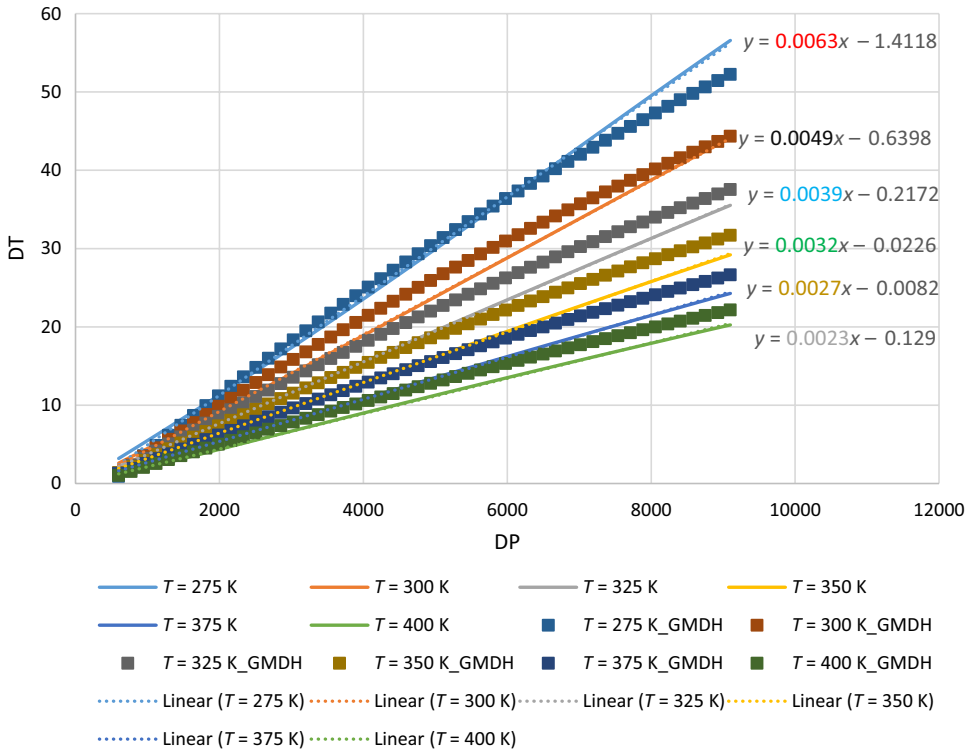


Fig. 11 Temperature drop across a JT valve for Sarkhon NG for various inlet temperatures by utilizing the GMDH method (output pressure is 900 kPa)

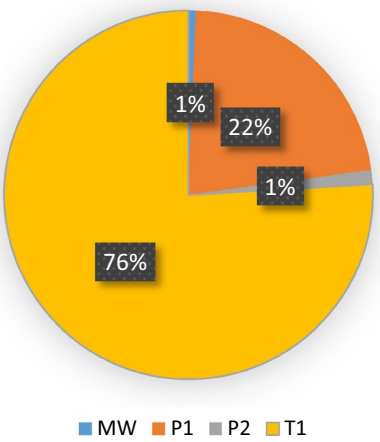


Fig. 12 Contribution of the important parameters on temperature drop across a JT valve

method, the temperature drop could be calculated much easier and faster than the MLP method.

The last but the most important findings are presented in Fig. 12. By analyzing the effects of each parameter on the temperature drop, the pie chart (Fig. 12) has been produced. Figure 12 shows the contribution of each important parameter on temperature drop across of a JT valve by utilizing machine learning (both MLP and GMDH methods). According to the pie chart, the contribution of the inlet temperature is 76%, the inlet pressure is 22%, the outlet pressure is 1% and the molecular weight is 1%. As shown in Fig. 12, the temperature drop across a JT valve has been mostly influenced by the inlet temperature and secondly inlet pressure. Consequently, the throttling process designers should mostly focus on inlet temperature as the most important parameter. The effects of natural gas compositions and outlet pressure on temperature drop across a JT valve could be neglected.

Conclusions

As direct prediction of temperature drop during the expansion process across a JT valve is usually not possible, in this work, artificial neural network method, specifically multilayer perceptron, is utilized to predict the temperature drop. Firstly, the GERG2008 EOS, as the most recent and authentic EOS for calculating natural gas thermodynamic properties, has been employed to produce a large database of natural gas thermodynamic properties for various mixtures. Then, this database along with available experimental data (totally 30,000 datasets) is utilized to train, validate and test the developed MLP network. In addition,

according to complexity of the multilayer perceptron model, a group method of data handling approach is used to simplify the major trained network. To train the GMDH neural network, 4000 randomized data that are generated by the main ANN-LMA neural network are utilized. These methods have been developed in a way to calculate the temperature drop across a JT valve directly. The results show that the direct temperature drop calculated with the two developed machine learning methods (MLP method and GMDH method) generated the error $R^2 = 0.998$ and $R^2 = 0.997$, respectively.

The effects of the four parameters (inlet temperature, inlet pressure, outlet pressure and natural gas compositions) on temperature drop across a JT valve have been studied. The results show that the inlet temperature is the most important parameter on temperature drop with a contribution of 76%. The inlet pressure with the contribution of 22% is the second most important parameter. The outlet pressure and natural gas compositions have negligible effects on temperature drop. The results also show that the temperature drop could be treated as a linear function of pressure drop where the slope is very close to the average JT coefficient.

Acknowledgments This research was partly funded by Iran National Science Foundation (INSF) under the contract no. 96004167 and Russian Foundation for Basic Research (RFBR Grant 17-58-560018). The second author would like to thank support from Ferdowsi University of Mashhad.

References

1. Cengel YA, Boles MA. Thermodyamics an engineering approach. New York: McGraw-Hill; 2002.
2. Sloan ED, Koh CA. Clathrate hydrates of natural gases, third edition. Clathrate Hydrates of Natural Gases. 2007.
3. Parvizi S, Arabkoohsar A, Farzaneh-Gord M. Natural gas compositions variation effect on capillary tube thermal mass flow meter performance. Flow Meas Instrum. 2016;50:229–36.
4. Kunz O, Wagner W. The GERG-2008 wide-range equation of state for natural gases and other mixtures: an expansion of GERG-2004. J Chem Eng Data. 2012;57:3032–91.
5. AGA8-DC92 EoS. Compressibility and super compressibility for natural gas and other hydrocarbon gases. Trans Meas Commun Rep 1992.
6. Ahmadi P, Chapoy A, Tohidi B. Density, speed of sound and derived thermodynamic properties of a synthetic natural gas. J Nat Gas Sci Eng. 2017;40:249–66.
7. Dranchuk PM, Abou-Kassem JH. Calculation of Z factors for natural gases using equations of state. J Can Pet Technol. 1975;14:34–6.
8. Londono FE, Archer RA, Blasingame TA. Correlations for hydrocarbon-gas viscosity and gas density-validation and correlation of behavior using a large-scale database. SPE Reserv Eval Eng. 2005;8:561–72.
9. AlQuraishi AA, Shokir EM. Viscosity and density correlations for hydrocarbon gases and pure and impure gas mixtures. Pet Sci Technol. 2009;27:1674–89.
10. Farzaneh-Gord M, Rahbari HR. Developing novel correlations for calculating natural gas thermodynamic properties. Chem Process Eng: Inz Chem I Process. 2011;32:435–52.
11. Farzaneh-Gord M, Farsiani M, Khosravi A, Arabkoohsar A, Dashti F. A novel method for calculating natural gas density based on Joule Thomson coefficient. J Nat Gas Sci Eng. 2015;26:1018–29.
12. Farzaneh-Gord M, Arabkoohsar A, Koury RNN. Novel natural gas molecular weight calculator equation as a functional of only temperature, pressure and sound speed. J Nat Gas Sci Eng. 2016;30:195–204.
13. Cao W, Wang X, Ming Z, Gao J. A review on neural networks with random weights. Neurocomputing. 2018;275:278–87.
14. Gill J, Singh J, Ohunakin OS, Adelekan DS. Component-wise exergy analysis using adaptive neuro-fuzzy inference system in vapor compression refrigeration system. J Therm Anal Calorim. 2019;136:2111–23.
15. Ramezanizadeh M, Alhuyi Nazari M, Ahmadi MH, Lorenzini G, Pop I. A review on the applications of intelligence methods in predicting thermal conductivity of nanofluids. J Therm Anal Calorim. 2019;138:827–43.
16. Ahmadpour J, Ahmadi M, Javdani A. Hydrodesulfurization unit for natural gas condensate. J Therm Anal Calorim. 2019;135:1943–9.
17. Ahmadi MH, Tatar A, Seifaddini P, Ghazvini M, Ghasempour R, Sheremet MA. Thermal conductivity and dynamic viscosity modeling of Fe_2O_3/water nanofluid by applying various connectionist approaches. Numer Heat Transf Part A Appl. 2018;74:1301–22.
18. Baghban A, Pourfayaz F, Ahmadi MH, Kasaeian A, Pourkiaei SM, Lorenzini G. Connectionist intelligent model estimates of convective heat transfer coefficient of nanofluids in circular cross-sectional channels. J Therm Anal Calorim. 2018;132:1213–39.
19. Maddah H, Aghayari R, Ahmadi MH, Rahimzadeh M, Ghasemi N. Prediction and modeling of MWCNT/Carbon (60/40)/SAE 10W 40/SAE 85W 90(50/50) nanofluid viscosity using artificial neural network (ANN) and self-organizing map (SOM). J Therm Anal Calorim. 2018;134:2275–86.
20. Ramezanizadeh M, Ahmadi MA, Ahmadi MH, Alhuyi Nazari M. Rigorous smart model for predicting dynamic viscosity of Al2O3/water nanofluid. J Therm Anal Calorim. 2019;137:307–16.
21. Ahmadi MH, Ahmadi MA, Nazari MA, Mahian O, Ghasempour R. A proposed model to predict thermal conductivity ratio of Al_2O_3/EG nanofluid by applying least squares support vector machine (LSSVM) and genetic algorithm as a connectionist approach. J Therm Anal Calorim. 2019;135:271–81.
22. Bagheri H, Behrang M, Assareh E, Izadi M, Sheremet MA. Free convection of hybrid nanofluids in a C-shaped chamber under variable heat flux and magnetic field: simulation, sensitivity analysis, and artificial neural networks. Energies. 2019;12:2807.
23. Moghadassi AR, Nikkholgh MR, Parvizian F, Hosseini SM. Estimation of thermophysical properties of dimethyl ether as a commercial refrigerant based on artificial neural networks. Expert Syst Appl. 2010;37:7755–61.
24. Kamyab M, Sampaio JHB, Qanbari F, Eustes AW. Using artificial neural networks to estimate the z-factor for natural hydrocarbon gases. J Pet Sci Eng. 2010;73:248–57.
25. Al-Anazi BD, Pazuki GR, Nikookar M, Al-Anazi AF. The prediction of the compressibility factor of sour and natural gas by an artificial neural network system. Pet Sci Technol. 2011;29:325–36.

26. Sanjari E, Lay EN. Estimation of natural gas compressibility factors using artificial neural network approach. J Nat Gas Sci Eng. 2012;9:220–6.
27. Mohamadi-Baghmolaei M, Azin R, Osfuri S, Mohamadi-Baghmolaei R, Zarei Z. Prediction of gas compressibility factor using intelligent models. Nat Gas Ind B. 2015;2:283–94.
28. Azizi N, Behbahani R, Isazadeh MA. An efficient correlation for calculating compressibility factor of natural gases. J Nat Gas Chem. 2010;19:642–5.
29. Mokhatab S, Poe WA. Handbook of natural gas transmission and processing. Burlington: Gulf Professional Publishing; 2012.
30. Farzaneh-Gord M, Arabkoohsar A, Deymi Dasht-bayaz M, Machado L, Koury RNN. Energy and exergy analysis of natural gas pressure reduction points equipped with solar heat and controllable heaters. Renew Energy. 2014;72:258–70.
31. ISO 20765-2—Natural gas—Calculation of thermodynamic properties—part 2: single-Phase properties (gas, liquid, and dense fluid) for extended ranges of application. 2015.
32. Hagan T, Demuth HB, Beale MH. Neural Network Design. 2002.
33. Kondo T. GMDH neural network algorithm using the heuristic self-organization method and its application to the pattern identification problem. Proceedings of SICE Annu Conference 1998. p. 1143–8.
34. Ernst G, Wirbser H, Keil B, Jaeschke M. Flow-calorimetric results for the massic heat capacity cp and the Joule-Thomson coefficient of CH4 of (0.85 CH4 + 0.15 C2H6) and of a mixture similar to natural gas. J Chem Thermodyn. 2001;33:601–13.
35. Day C, Stephan M, Oellrich LR. A new flow calorimeter for the measurement of the isobaric enthalpy increment and the isenthalpic Joule–Thomson effect. Results for methane and (methane + ethane). J Chem Thermodyn. 1997;29:949–71.
36. National Iran Gas Company official website. Available from: http://nigc.com/pages/Products.html.