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Accurate determination of natural gas compressibility factor by measuring temperature, pressure and Joule-Thomson coefficient: Artificial neural network approach

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ABSTRACT

Natural Gas (NG) compressibility factor as important property at any NG industrial applications determined by utilizing an intelligent approach precisely. Three thermodynamic properties include pressure, temperature and Joule-Thomson (JT) coefficient are selected as input parameters. These properties are chosen due to the measurement capabilities of available sensors. Unlike the traditional approaches, the current approach does not require NG compositions as input. The current intelligent approach is developed based on an Artificial Neural Network (ANN) method. Real-time measurement capability and very low cost are two main advantages of the developed approach. Big data sets of NG thermodynamic properties are created considering 30,000 random compositions for training, testing and validating the ANN. The GERG-2008 is utilized (as the most recent equation of state) to calculate thermodynamic properties to train the ANN. Validation of the developed ANN method compared to experimental data shows the Average Absolute Percent Deviation (AAPD) is about 0.33%. To show the accuracy of the developed approach, four different NG compositions are selected as case studies. The compressibility factor and JT coefficient are computed for various pressure and temperature range using the traditional approach. Then, the compressibility factor is determined using the intelligent approach when only pressure, temperature and JT coefficient are known. The AAPD of NG compressibility factor calculations for various natural gases show 0.385% for pure methane, 0.45% for the Khangiran gas, 0.58% for the Kangan gas, 0.78% for the Pars gas and is 1.12% for the Bidboland gas. The comparing results show that overall AAPD is less than 0.7% that shows the high accuracy of the intelligent approach.

1. Introduction

1.1. Motivation

Natural Gas (NG) compressibility factor is widely used in NG industries such as NG flow measurement stations (Hiismaeki, 1993; Smalling et al., 1989). The NG compressibility factor is especially required in flow metering stations for calculating NG mass flow rate (Froysa and Lunde, 2005, 2011). The compressibility factor is also the main input for calculating other thermodynamic properties. The compressibility factor is traditionally are calculated with low accuracy using empirical correlation and with high accuracy using Equations of States (EOS).

1.2. Literature

The most important and useful empirical correlations can be found in various researches (Hirschfelder et al., 1955), (Watson and White, 1982), (Valdes and Cadet, 1991), (Dell'Isola et al., 1997), (Buonanno et al., 1998) and (Hammond, 2001). Due to the simplicity of empirical correlations, these equations are utilized frequently in the NG process simulation as well as the NG thermodynamic properties determination. In recent years, researchers have presented many empirical correlations with acceptable accuracy. The empirical correlations whose main objective is to compute the NG compressibility factor can be referred to (Azizi et al., 2010; Bahadori et al., 2007; Dranchuk and Abou-Kassem, 1975; Elsharkawy, 2004; Hall and Holste, 1995; Heidaryan et al, 2010a, 2010b). The most important recent studies in this field are: a set

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Nomenclature

f	Activation function
T	Temperature(K)
P	Pressure(kPa)
J	Jacobian matrix
Z	Z-factor
X	Mole fraction
v	Gas volume
α	Helmholtz free energy
δ	Reduced fluid mixture
$\beta_{v,ij}, \gamma_{T,ij}, \beta_{T,ij}, \gamma_{T,ij}$	Binary mixtures parameters of GERG-2008 EOS
α^0	Helmholtz free energy ideal part of the gas mixture
α^0_{0i}	Ideal dimensionless Helmholtz free energy of 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 $\left(\frac{1}{K}\right)$
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
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

B	Base condition
C	Critical point
F	Flow condition
R	Reduced

Abbreviation

AAPD	Average Absolute Percent Deviation
ANN	Artificial Neural Network
CF	Correction Factor
EOS	Equations of State
HFE	Helmholtz Free Energy
JT	Joule-Thomson Coefficent
NG	Natural Gas
MLP	Multilayer perceptron
RMSE	Root Mean Squares of Error

of correlations for computing NG thermodynamic properties (i.e. compressibility factor) that presented by Farzaneh-Gord and Rahbari (2011). Fayazi et al. (2014) introduced the accurate model to predict sour and sweet NG Z-factor (i.e. compressibility factor). In their study, a new approach was proposed to predict the NG compressibility factor using a large database of 2000 samples. The results of their study show that their proposed model reported an error of 0.19%, as compared to other correlations. In all the empirical correlations mentioned above, for calculating the NG compressibility factor, it is necessary to know the temperature, pressure as well as NG compositions (i.e. NG molecular weight). It should be pointed out that, empirical correlations are not usually used in NG measurement processes because of their low accuracy.

EOSs are widely used for calculating NG thermodynamic properties such as the compressibility factor. Two equations of AGA8 and GERG-2008 have developed especially for NG by NG industries. They show high accuracy and are accepted as standard methods for calculating the NG compressibility factor. Considering the high accuracy of these EOSs, the ISO20765-1 (ISO 20765-1, 2005) standard is developed based on AGA8 EOS (AGA8-DC92 EoS, 1992) and ISO20765-2 (ISO 20765-2, 2015) based on GERG-2008 EOS (Kunz and Wagner, 2012). According to the description, these EOS utilized for computing NG flow at custody transfer points. In recent years, researches have been carried out to calculate the thermodynamic properties of natural gas based on these EOSs. Marić et al. (2005) calculated NG isentropic exponent based on AGA8 EOS. Also, the Joule-Thomson (JT) coefficient and the heat capacity of NG were calculated using extended AGA8 EOS by Marić (Marić, 2005, 2007). Farzaneh-Gord et al. (2010) and Farzaneh-Gord and Rahbari (2012) developed AGA8 EOS and presented methods and procedures for computing other thermodynamics properties of NG such as the speed of sound, entropy, enthalpy and internal energy. Also, Farzaneh-Gord et al. (2018) were compared the sensitivity of AGA8 EOS and GERG-2008 EOS in the calculation of NG flow measurement. In their study, the NG compressibility factor was computed based on both these two EOSs. The results of their study were shown that the accuracy of GERG-2008 EOS is higher than AGA8 EOS. It should be pointed out that, to calculate the NG compressibility factor, using these two EOSs, the temperature, pressure and NG compositions should be known.

Generally, NG temperature and pressure could be easily measured but the measurement of NG compositions is an expensive process and is a very difficult procedure. Therefore, real-time NG mixture compositions measurement are not usually carried out. For example, in Iran as the case study of this work, the composition measurements usually carried out yearly in metering stations. To overcome this issue, the researchers proposed methods for the NG molecular weight using three measurable NG thermodynamic properties. The first study, in this case, was presented by Farzaneh-Gord et al. (Farzaneh-Gord et al, 2015, 2016) such that in these studies, the NG thermodynamic properties are calculated based on three measurable properties. Farzaneh-Gord et al. (2016) presented a novel correlation to calculate NG molecular weight based on three measurable properties including temperature, pressure and speed of sound. The results of their study were shown that the developed correlation is calculated NG molecular weight with acceptable accuracy. In addition, Farzaneh-Gord et al. (2015) developed a novel method to compute the NG density based on temperature, pressure and JT coefficient as three measurable thermodynamic properties. The results of their study were shown that the error in the density calculation is not more than 1.2%. Researchers have considered the calculation of the NG thermodynamic properties using three measurable properties in recent years. For example, Khosravi et al. (2018) utilized several artificial intelligence approaches to predict the density of NG based on temperature, pressure and JT while using AGA8 EOS to train network data. In one study, Liu et al. (2019) calculated the NG compressibility factor based on pressure, temperature and volume as three measurable properties. Their results were shown that the error in calculating the NG compressibility factor does not exceed 2.1%.

Researchers for calculating the thermodynamic properties of NG in recent years proposed artificial Neural Network (ANN) methods. For example, Sanjari and Nemati (Sanjari and Lay, 2012) presented an ANN based on the back-propagation method to predict the NG compressibility

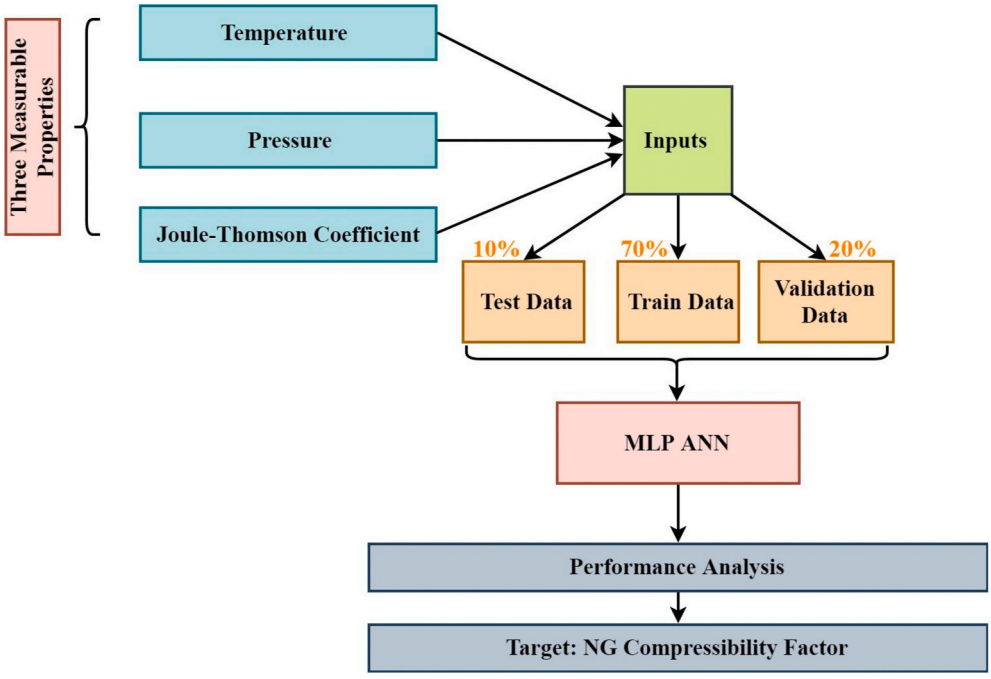

Fig. 1. Procedure of NG compressibility factor calculation proposed in this study.

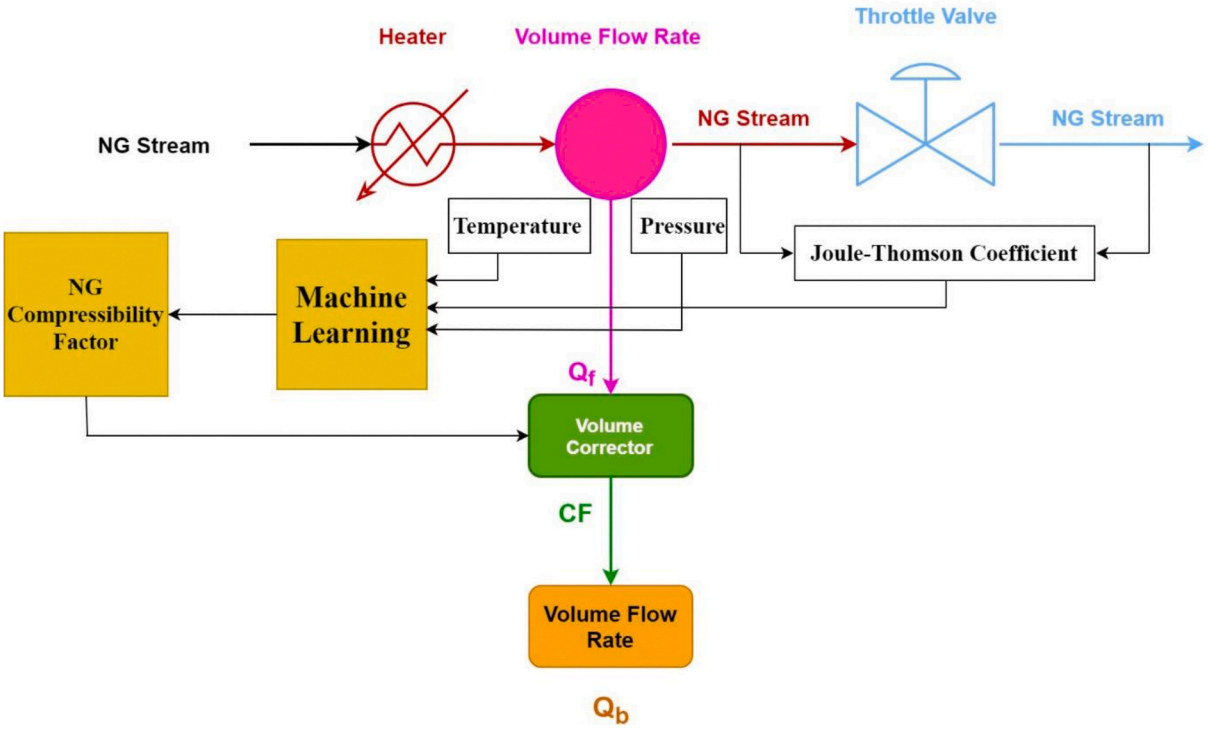

Fig. 2. A typical pressure drop station along with flow metering instrument.

factor. In their study, about 5500 compressibility factors experimental data were employed for training and testing of ANN. The results of their study were compared to Peng-Robinson EOS that their calculations had an error equivalent to 0.6%. Chamkalani et al. (2013) developed a machine learning method to calculate the NG compressibility factor. The least square support vector machine was utilized in their work and their results were shown a correlation coefficient of about 0.999 and MSE about 0.000014 compared to previous models. Ghiasi et al. (2014) developed a robust modeling approach to estimate the compressibility factor for gas condensates. Their model was compared to 120 previous models and the results were shown that the proposed model has high accuracy toward all the studied methods. Kamari et al. (2016) presented a corresponding states-based method to predict the NG compressibility factor. Their proposed model is more accurate compared to other models. Rebai et al. (2019) predicted the NG hydrates formation conditions using a combination of thermodynamic and ANN modeling. They

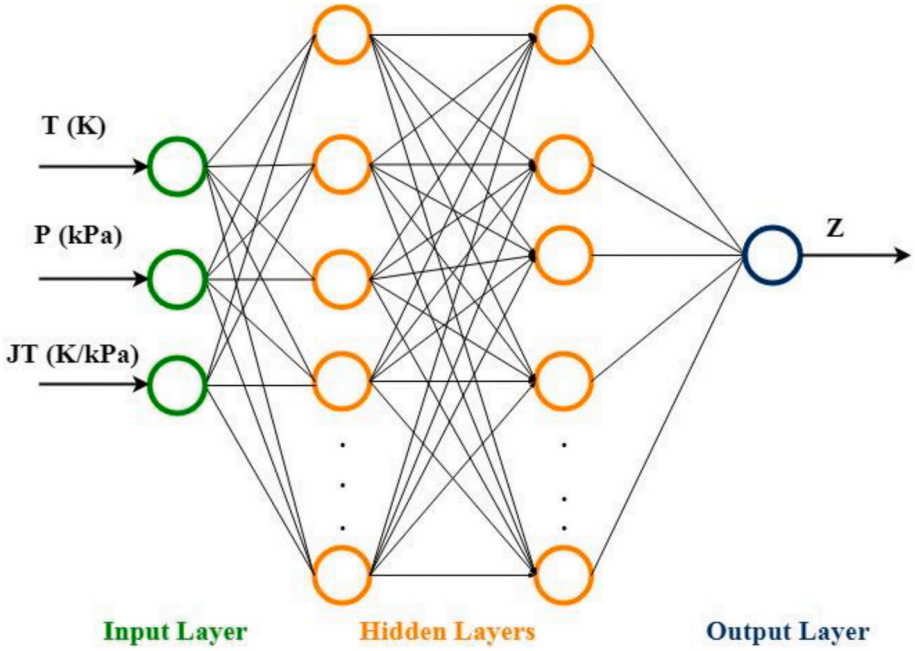

Fig. 3. Structure of the proposed MLP ANN.

Table 1
The detailed report of the proposed MLP ANN.

Parameter	Value/Comment
Number of inputs layer neurons	3
Number of Hidden Layers	4
Neurons' number in each Hidden layers	19
Activation function of hidden layers	Tansig
Activation function of Output layers	Purelin
Total data used in each ANN complex	29,871
Train data percent	70%
Validation data percent	15%
Test data percent	15%
Correlation coefficient of output [T]	0.99999
Correlation coefficient output [Z]	0.99999
Best validation performance at Epoch	600

used a database of 4660 data points to validate the proposed model. Their results show that the proposed model predicts the hydrates formation conditions with high precision compared to previous models. In a recent study, Azizi et al. (2019) presented an intelligent approach to predict the NG compressibility factor based on ANN. Their model is optimized to achieve high precision. Their study shows their model is an accurate method for the calculation of the NG compressibility factor.

1.3. Objective and novelty

The current study presents an intelligent approach for calculating NG thermodynamic properties without any knowledge of its composition. Unlike the previous studies, the proposed method has been developed so that to calculate the compressibility factor with high accuracy. The current approach could be employed even for custody transfer purposes. To developed the approach, firstly, two thermodynamics properties (JT coefficient and compressibility factor) are calculated for wide temperature and pressure range for 30,000 random data sets of compositions using GERG-2008 EOS. Based on these data sets of four thermodynamics properties (temperature, pressure and JT coefficient and compressibility factor), an ANN is developed in a way to compute NG compressibility factor using the other three properties as input (pressure, temperature and JT coefficient). Due to the low cost of real-time measuring of these three properties, the current study presents a cost-effective method for real-time measuring of compressibility factor precisely. Fig. 1 illustrates how the proposed method operates.

2. Methodology

2.1. The developed approach sample application

The developed approach could have enormous applications in NG industries especially in places where real-time properties are needed. In this section, a sample application is given. Fig. 2 represents a typical NG pressure drop and measuring station with flow metering instruments. As seen in Fig. 2, temperature, pressure and JT coefficient (i.e. NG properties) could be measured in the metering station.

At NG custody transfer points, the NG volume flow rate at the base condition is needed. This parameter can be calculated as follow (Mokhatab and Poe, 2012):

$$Q_b = CF \times Q_f \tag{1}$$

In which,CF is the correction factor, Q_b is the volume flow rate in base condition and Q_f is the volume flow rate in flow conditions (measured with a volume flow meter). The correction factor is calculated by the following equation (Mokhatab and Poe, 2012):

$$CF = \left(\frac{T_b}{T_f}\right)\left(\frac{P_f + P_{atm}}{P_b}\right)\left(\frac{Z_b}{Z_f}\right) \tag{2}$$

In the above equation, T, P and Z are the temperature, pressure and compressibility factor of NG respectively. Also, the subscript f, b and atm refer to the flow condition, base conditions and ambient conditions respectively. As mentioned, the accurate calculation of the compressibility factor at the NG metering stations (particularly at big stations) is very important. Both ISO20765-1 and ISO20765-2 require NG compositions as input to calculate the NG compressibility factor. The NG composition measurement needs additional and very expensive instruments that are not feasible to install in all metering stations.

The current approach eliminates the need for knowing NG composition in these stations. As temperature and pressure could be measured easily across the throttling valve, consequently, the JT coefficient could be computed. By knowing three properties (pressure, temperature and

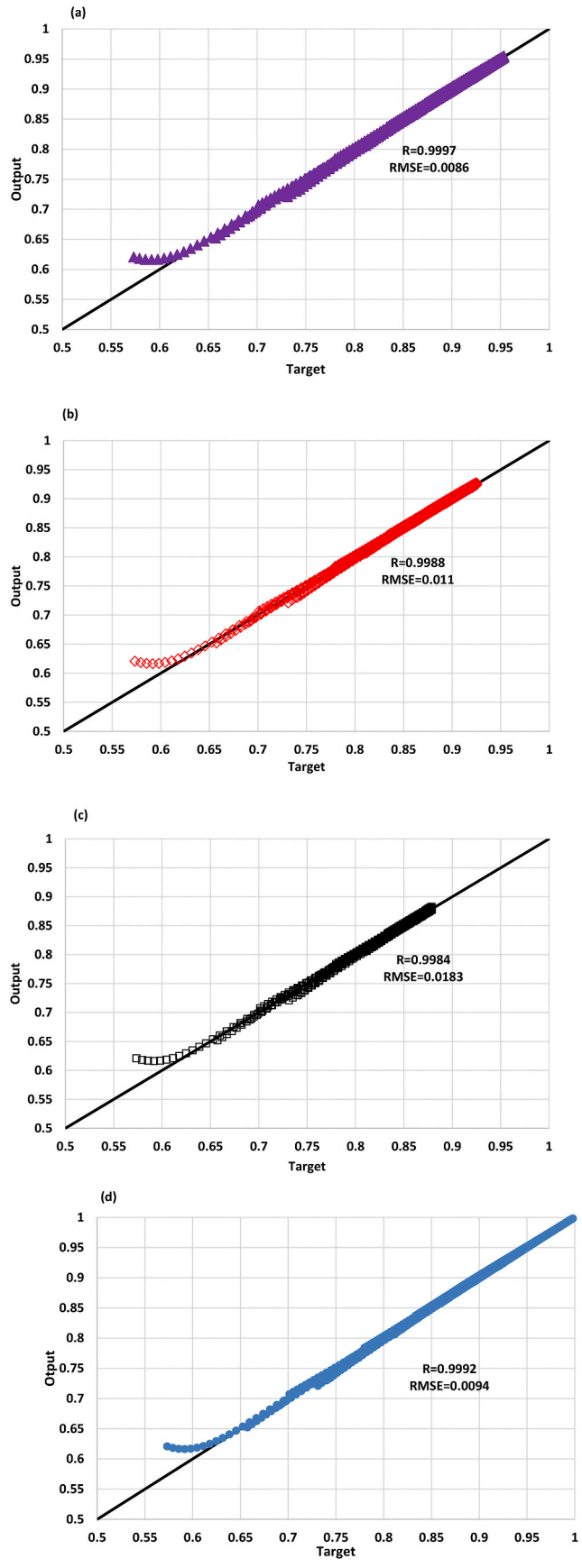

Fig. 4. NG Compressibility factor ANN outputs versus target data for (a) train data, (b) validation data, (c) test data and (d) all of the used data.

Table 2
The mole fraction of Synthetic NG mixture (Nasrifar and Bolland, 2006).

Component	Mole fraction
CH_4	0.79942
C_2H_6	0.05029
C_3H_8	0.03
N_2	0.09939
CO_2	0.0209

JT coefficient) and utilizing the proposed intelligent approach, one could determine the compressibility factor and consequently CF.

2.2. ANN approach

The proposed ANN approach for calculating the NG compressibility factor is developed in this section. Firstly, a database of temperature, pressure and JT coefficient and compressibility factor for various NG composition is constructed. Due to limited experimental values, here, most data are obtained by solving a widely accepted EOS. Based on the information given by Farzaneh-Gord et al. (2018), the GREG-2008 EOS (Kunz and Wagner, 2012) has been selected as the EOS for calculating NG thermodynamics properties. For this purpose, 30,000 random datasets of NG compositions are selected based on the rage of NG component for pipeline gas quality (ISO 20765-2, 2015). A few available experimental combinations of these four properties are also added to the database. Finally, using the sub-model of Artificial Neural Network (here, multilayer perceptron), an ANN is trained and structured in a way to calculate the compressibility factor by three inputs (temperature, pressure and JT coefficient).

2.3. Computing compressibility factor using GERG-2008

Helmholtz's free energy definition is the starting point for developing GERG-2008 EOS. For a mixture, the Helmholtz free energy as a function of density, ρ, temperature, T and compositions,$\overline{X}$, is defined as following (Kunz and Wagner, 2012):

$$a\left(\rho,T,\overline{X}\right)=a^0\left(\rho,T,\overline{X}\right)+a^r\left(\rho,T,\overline{X}\right) \tag{3}$$

where, a^0 *and* a^r are the ideal part and reduce part of the gas mixture respectively. Unlike most EOSs, the EOS takes density and temperature as the independent variables (not temperature and pressure). The pressure is calculated by an iterative technique. Assuming, $=\frac{a}{RT}$, the above equation could be rewritten as follow (Kunz and Wagner, 2012):

$$\alpha\left(\delta,\tau,\overline{X}\right)=\alpha^0\left(\rho,T,\overline{X}\right)+\alpha^r\left(\delta,T,\overline{X}\right) \tag{4}$$

In which, δ *and* τ are reduced fluid mixture density and inverse reduced temperature respectively.

Theδ and τ are expressed as $\delta=\frac{\rho}{\rho_r(x_i)}$ and $\tau=\frac{T_r(x_i)}{T}$ where $T_r(x_i)$*and* $\rho_r(x_i)$ are calculated as (Kunz and Wagner, 2012):

$$\frac{1}{\rho_r\left(\overline{X}\right)}=\sum_{i=1}^{N}\sum_{j=1}^{N}X_iX_j\beta_{v,ij}\gamma_{v,ij}\frac{X_i+X_j}{\beta_{v,ij}^2x_i+x_j}\left[\frac{1}{8}\right]\left(\frac{1}{\rho_{c,i}^{1/3}}+\frac{1}{\rho_{c,j}^{1/3}}\right)^3 \tag{5}$$

$$T_r\left(\overline{X}\right)=\sum_{i=1}^{N}\sum_{j=1}^{N}X_iX_j\beta_{T,ij}\gamma_{T,ij}\frac{X_i+X_j}{\beta_{T,ij}^2X_i+X_i}\left(T_{c,i}.T_{c,j}\right)^{0.5} \tag{6}$$

In equation (5) and (6), ρ_r and T_r are a function of the NG compositions. The detailed information for the parameters used in equation (5) and (6) could be found in ISO 20765–2 (Kunz and Wagner, 2012).

The ideal part of Helmholtz free energy, in equation (4), could be defined by the following equation (Kunz and Wagner, 2012):

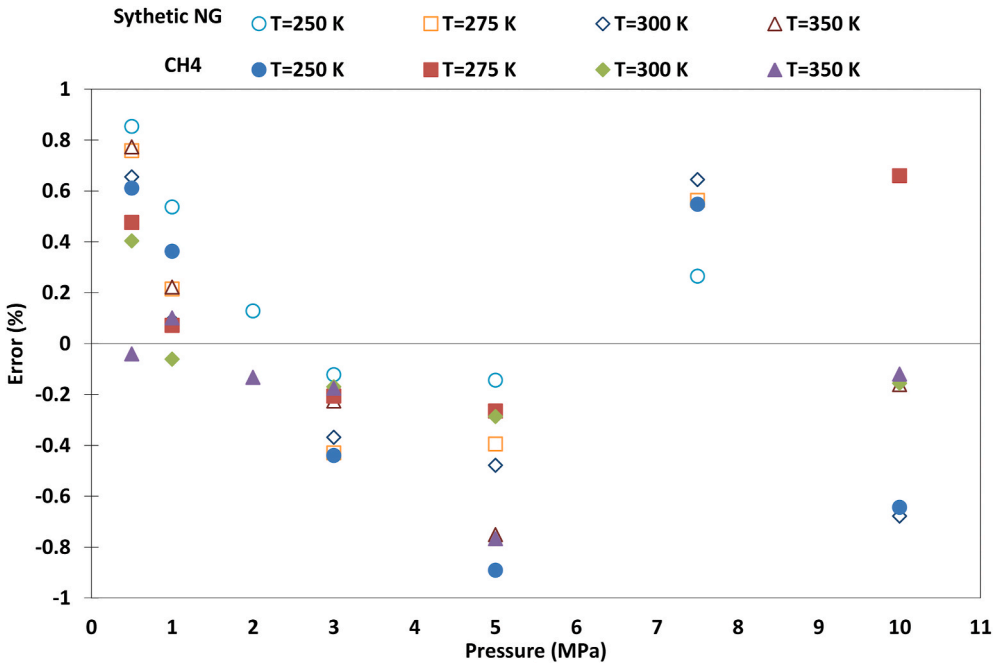

Fig. 5. The error present of MLP ANN versus pressure on the constant temperature for pure methane and a Synthetic NG.

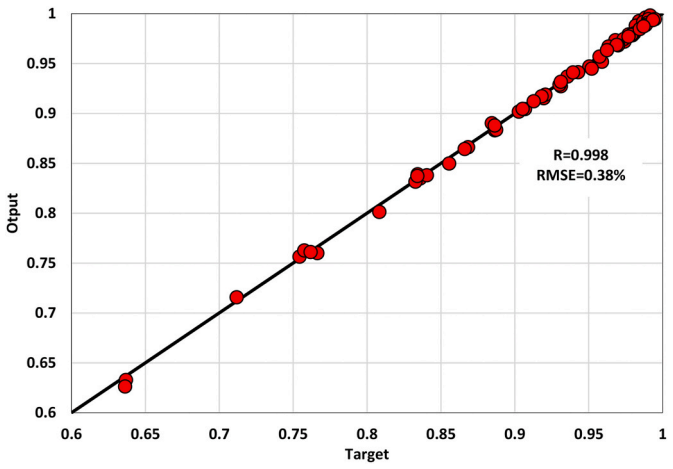

Fig. 6. Output MLP ANN Z-factor versus target Z-factor from (Nasrifar and Bolland, 2006).

Table 3
The mole fraction of natural gases from Iran's fields ("National Iran Gas Company official website.").

Component	Khangiran	Kangan	Pars	Bidboland
CH_4	0.98548	0.8802	0.87	0.8501
N_2	0.005	0.0545	0.031	0.0044
CO_2	0	0	0.0171	0.0041
C_2H_6	0.00647	0.0413	0.054	0.0938
C_3H_8	0.00069	0.0129	0.017	0.0349
i-C_4H_{10}	0.00018	0.0028	0.003	0.0034
n- C_4H_{10}	0.00039	0.0038	0.0045	0.0065
i- C_5H_{12}	0.00018	0.0016	0.0013	0.001
n- C_5H_{12}	0.00021	0.001	0.0011	0.0009
n-C_6H_{14}	0.0014	0.0019	0.0007	0.0009
C_7^+	0	0	0.0003	0
Molecular Weight	**16.43**	**17.79**	**18.68**	**18.86**

$$\alpha^0\left(\rho,T,\overline{X}\right)=\sum_{i=1}^{N}X_i\left[\alpha_{0i}^0(\rho,T)+Ln(X_i)\right] \tag{7}$$

In which, $\alpha_{0i}^0(\rho,T)$ and $\sum X_i Ln(X_i)$ are the ideal dimensionless Helmholtz free energy and entropy production due to the mixing of component i, respectively.

The residual part of Helmholtz free energy, in equation (4), could be calculated as below (Kunz and Wagner, 2012):

$$\alpha^r\left(\delta,\tau,\overline{X}\right)=\alpha_0^r\left(\delta,\tau,\overline{X}\right)+\Delta\alpha^r\left(\delta,\tau,\overline{X}\right) \tag{8}$$

where, α_0^r is the generalized departure function and $\Delta\alpha^r$ is the specific departure function.

The generalized departure function, α_{or}^r, stands for pure substances residual contribution and could be computed as (Kunz and Wagner, 2012):

$$\alpha_0^r\left(\delta,\tau,\overline{X}\right)=\sum_{i=1}^{N}X_i\alpha_{0i}^r(\delta,\tau) \tag{9}$$

The $\Delta\alpha^r$ is the specific departure function. This function is the double summation of all binary specific and generalized departure functions developed for the binary subsystems and could be defined as (Kunz and Wagner, 2012):

$$\Delta\alpha^r\left(\delta,\tau,\overline{X}\right)=\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\Delta\alpha_{ij}^r\left(\delta,\tau,\overline{X}\right) \tag{10}$$

with:

$$\Delta\alpha_{ij}^r\left(\delta,\tau,\overline{X}\right)=X_iX_jF_{ij}\alpha_{ij}^r(\delta,\tau) \tag{11}$$

In the above equations, $F_{ij}$is the EOS parameters and $\alpha_{ij}^r(\delta,\tau)$ is temperature and density dependence of specific departure functions. $\alpha_{ij}^r(\delta,\tau)$ was developed either for a specific binary mixture (a binary specific departure function with binary specific coefficients and exponents) or for a group of binary mixtures generalized departure function with a uniform structure for the group of binary mixtures). It could be calculated as below (Kunz and Wagner, 2012):

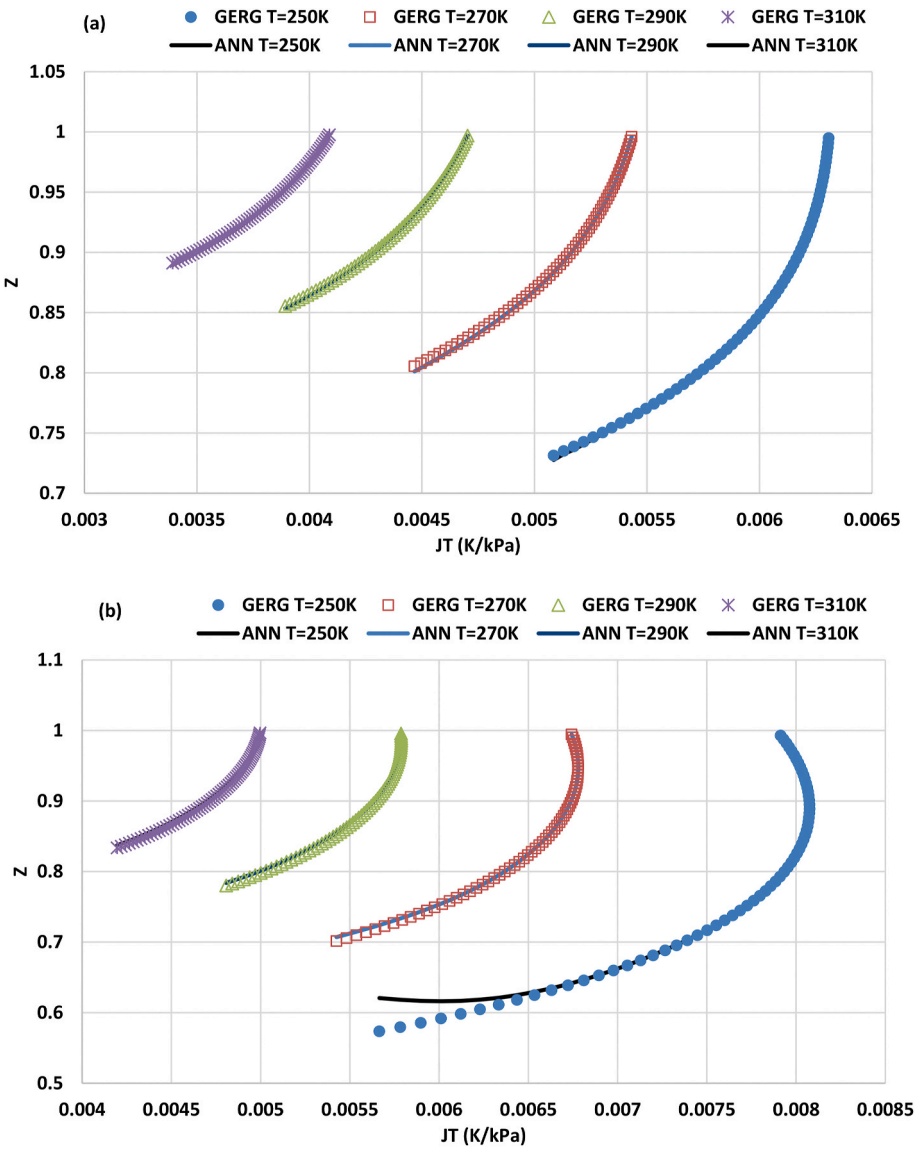

Fig. 7. The compressibility factor versus JT in the constant temperatures for studied natural gases: (a) Khangiran and (b) Bidboland.

$$\alpha_{ij}^{r}(\delta,\tau)=\sum_{k=1}^{K_{Pol,ij}} n_{ij,k}\delta^{d_{ij,k}}\tau^{t_{ij,k}}+\sum_{K=K_{Pol,ij}+1}^{K_{Pol,ij}+K_{Exp,ij}} n_{ij,k}\delta^{d_{ij,k}}\tau^{t_{ij,k}}e^{-\eta_{ij,k}\left(\delta-\varepsilon_{ij,k}\right)^{2}-\beta_{ij,k}\left(\delta-\gamma_{ij,k}\right)} \tag{12}$$

The coefficients$n_{ij,k}$, $d_{ij,k}$ and $t_{ij,k}$, $\eta_{ij,k}$, $\varepsilon_{ij,k}$, $\beta_{ij,k}$, and $\gamma_{ij,k}$ are the EOS parameters and constant. They could be found in ISO 20765–2.

Finally, the NG compressibility factor in GERG-2008 EOS could be computed as follow (Kunz and Wagner, 2012):

$$Z=1+\delta\alpha_{\delta}^{r} \tag{13}$$

where, α_{δ}^{r} is calculated by the following equations (Kunz and Wagner, 2012):

$$\alpha_{\delta}^{r}=\left(\frac{\partial a_{r}}{\partial\delta}\right)_{\tau,X} \tag{14}$$

As NG pressure and temperature along with NG compositions are measured, the density is guessed at the first step and then by employing an iterative technique the pressure will be found. The other properties including Z will be calculated afterward. There are two ranges for using the GERG-2008 EOS (Kunz and Wagner, 2012): the normal and extended range. In the normal range, the temperature is between 90 K and 450 K and the pressure is up to 35,000 kPa. In addition, in the extended range, the temperature is between 60 K and 700 K and the pressure is valid up to 70,000 kPa.

2.4. Computing Joule-Thomson coefficient using GERG-2008 EOS

The calculations of NG thermodynamic properties such as the JT coefficient are related to derivatives of the Helmholtz free energy with respect to the reduced mixture variables δ and τ. All of the thermodynamic properties may be written explicitly in terms of the reduced Helmholtz free energy α and its various derivatives. The required derivatives to calculated thermodynamic properties are given below (Kunz and Wagner, 2012):

$$\alpha_{\delta}=\left(\frac{\partial\alpha}{\partial\delta}\right)_{\tau,\overline{X}},\alpha_{\delta\delta}=\left(\frac{\partial^{2}\alpha}{\partial\delta^{2}}\right)_{\tau,\overline{X}},\alpha_{\tau}=\left(\frac{\partial\alpha}{\partial\tau}\right)_{\tau,\overline{X}},\alpha_{\tau\tau}=\left(\frac{\partial^{2}\alpha}{\partial\tau^{2}}\right)_{\delta,\overline{X}},$$
$$\alpha_{\tau\delta}=\left[\frac{\partial}{\partial\tau}\left(\frac{\partial\alpha}{\partial\delta}\right)_{\tau,X}\right]_{\delta,\overline{X}} \tag{15}$$

The JT coefficient, JT, is calculated in GERG-2008 EOS by employing the following equation (Kunz and Wagner, 2012):

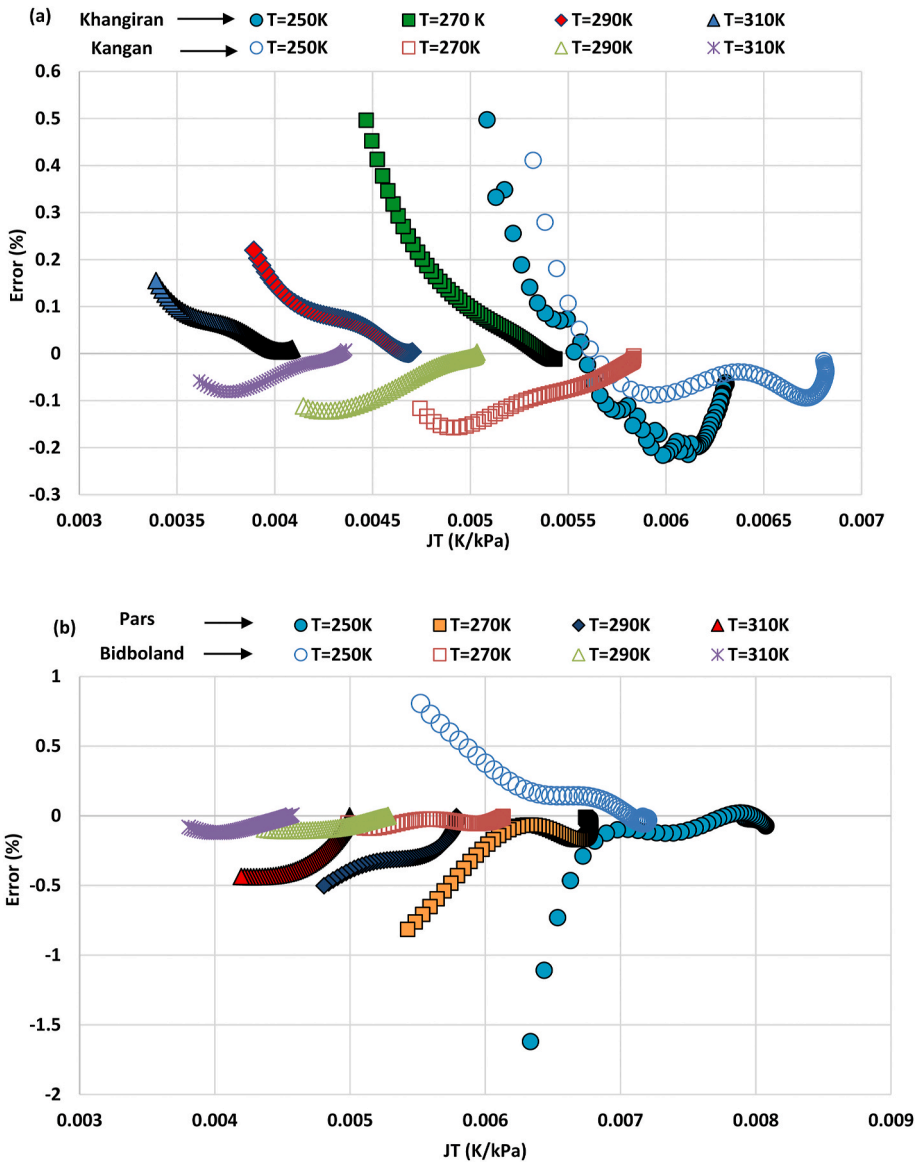

Fig. 8. The compressibility factor error calculation versus JT in the constant temperatures for studied NG mixture: (a) Khangiran and Kangan and (b) Pars and Bidboland.

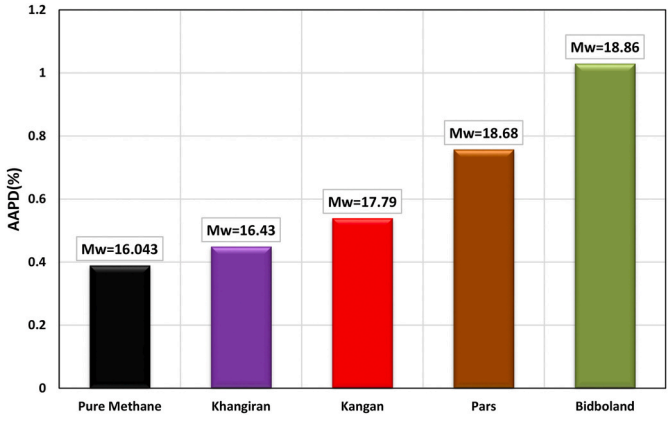

Fig. 9. AAPD of the NG compressibility factor calculation for various natural gases.

$$JT = \left(\frac{\partial T}{\partial P}\right)_{h,\bar{X}} = \frac{\alpha_2 - \alpha_1}{\alpha_2^2 - (\tau^2.\alpha_{\tau\tau}.\alpha_1)} = \frac{R}{c_p}\left(\frac{\alpha_2}{\alpha_1} - 1\right) = \frac{R}{c_p.M}\left(\frac{\alpha_2}{\alpha_1} - 1\right) \quad (16)$$

The reduced Helmholtz free energy derivatives in the above equation (i.e. α_1 and α_2) could be defined as the following equations (Kunz and Wagner, 2012):

$$\alpha_1 = \left[\frac{\partial(\delta^2\alpha_\delta)}{\partial\delta}\right]_{\tau,\bar{X}} = 2\delta\alpha_\delta + \delta^2\alpha_{\delta\delta} \quad (17)$$

$$\alpha_2 = -\tau^2\left[\frac{\partial}{\partial\tau}\left(\frac{\delta\alpha_\delta}{\tau}\right)\right]_{\delta,\bar{X}} = \delta\alpha_\delta - \tau\delta\alpha_{\tau\delta} \quad (18)$$

In equation (16), M is molecular weight, $R$is the molar gas constant and c_p is the isobaric heat capacity.

2.5. MLP method

Artificial Neural Network (ANN) is an efficient algorithm for handling data with many discontinuities. The basic principles of ANN that are designed based on the human brain are learning the relationship

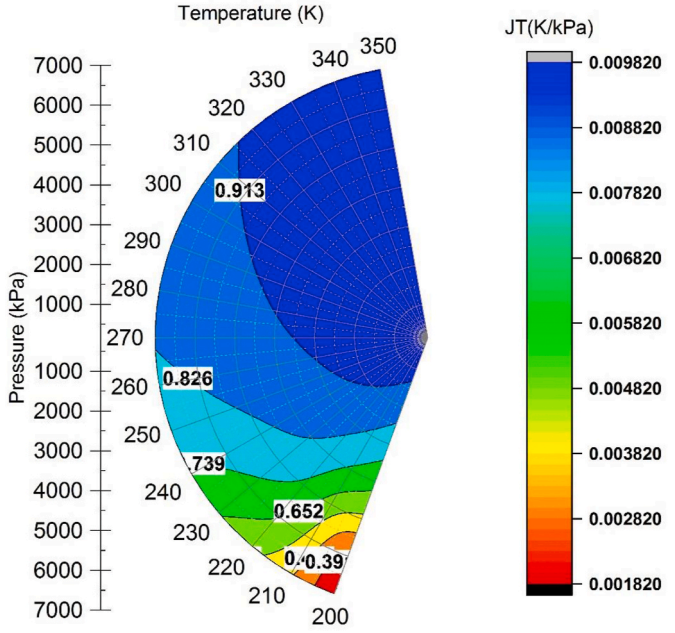

Fig. 10. The polar plot of the NG compressibility factor versus temperature, pressure and JT coefficient.

between the input and output of the network by utilizing trial and error (T.Hagan et al., 2002). The multilayer perceptron (MLP) model is one of the most basic ANN which is used to simulate the transmission function of the human brain. In this type of neural network, most of the network behavior of the human brain and signal propagation is considered and hence, it is sometimes referred to as the feed-forward networks. Each neuron (as the neural cell of the human brain) performs the processing of input and then transfers the result to another cell. This continues to get an outcome that will finally lead to a decision. (T.Hagan et al., 2002). The input layer, the hidden layer and the output layer are three layers, which are forming the MLP ANN. The independent variables in the problem are input layer neurons. It is the task of latent layer neurons to make connections between independent and dependent variables. The dependent variables are present in the output layer neurons. The main components of an MLP ANN include the algorithms for training the networks, the weights, the biases and the data collected for training. One of the parameters in the ANN is called an Activation function. The Activation function is a mathematical equation that determines the output of a neural network. The tangential hyperbolic (tansig) function is used as an activation function in the hidden layer. Also, the activation functions utilized in the output layer is a linear function (T.Hagan et al., 2002). These Activation functions defined by the following equation:

$$f(a) = \tanh(a) = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)} \; ; [-1, 1] \text{ (tangential hyperbolic function)} \tag{19}$$

$$f(a) = a \; ; (-\infty, \infty) \text{ (linear function)} \tag{20}$$

An algorithm should be trained in the neural network data. There are varieties of training algorithms for this purpose. In this study, the Levenberg-Marquadt learning algorithm is used for training the proposed MLP ANN. Levenberg-Marquadt is one of the powerful Back-propagation learning algorithms. The main duty of Levenberg-Marquadt is the optimization of weights and biases that is obtained by using the following equation (T.Hagan et al., 2002):

$$W^{(k+1)} = W^{(k)} - \left(\left[J^T.J + \mu I \right]^{-1} \right).(J^T.e) \tag{21}$$

In equation (21), *W*, *J*, *e and I* are weighted matrix, Jacobian Matrix, output/its target difference and *I* diagonal matrix which formed the main diagonal of J^TJ, respectively.

In this study, the temperature, pressure and JT coefficient are input parameters of the MLP ANN. These parameters are three measurable properties that are required to calculate the NG compressibility factor. The model output parameters can consist of several thermodynamic and physical properties, including the NG compressibility factor. Fig. 3 reveals the structure of the proposed MLP model including input, hidden and output parameters. Also, the detailed information of the proposed MLP ANN are reported in Table 1.

2.6. Assessment of the developed ANN

In this section, two important parameters are defined to determine the performance of the developed ANN. The first parameter is the root mean sum of squares of the errors (RMSE) that defined as follow (T. Hagan et al., 2002):

$$RMSE = \frac{1}{N} \sum_{i=1}^{N} (t_i - a_i)^2 \tag{22}$$

The correlation coefficient for each input data, *R*, as the second parameter, could be determined as follow (T.Hagan et al., 2002):

$$R = \frac{N\left(\sum_{i=1}^{N} a_i t_i\right) - \left(\sum_{i=1}^{N} a_i\right)\left(\sum_{i=1}^{N} t_i\right)}{\sqrt{N\sum_{i=1}^{N} a_i^2 - \left(\sum_{i=1}^{N} a_i\right)^2}\sqrt{N\sum_{i=1}^{N} t_i^2 - \left(\sum_{i=1}^{N} t_i\right)^2}} \tag{23}$$

In the above equations, *N,t and a* are the total number of training data, the target value and the network output value respectively.

In addition, to validate the MLP method with other methods (here GERG-2008 EOS), two parameters have been defined. The first parameter is the percentage error defined by the following equation:

$$ERROR = \left| \frac{\hat{y}_i - y_i}{y_i} \right| \times 100\% \tag{24}$$

The second parameter is the average absolute percent deviation (AAPD) that defined as follow (Chamkalani et al., 2013):

$$AAPD = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\hat{y}_i - y_i}{y_i} \right| \times 100\% \tag{25}$$

In equations (24) and (25), ŷ and y are the estimated and observed values of the NG compressibility factor. Also, N is the total data used in the validation procedure.

Given the characteristics of the developed MLP ANN, which are listed in Table 1, 70%, 15% and 15% of all data respectively are used for training, validation and testing of MLP ANN. Fig. 4 shows the output NG compressibility factor versus target data for training, validation, testing and all data set of the proposed MLP ANN. According to equations (22) and (23), the values of RMSE for the compressibility factor calculation is 0.0086, 0.011, 0.0183, 0.0094 and the values of R is 0.9997,0.9988, 0.9984, 0.9992 for training data, validation data, testing data and all data, respectively. According to the results obtained from Fig. 4 as well as the RMSE and R values, the proposed MLP ANN predicts the compressibility coefficient as a function of temperature, pressure and JT coefficient with high precision.

3. Results and discussion

3.1. Validating the MLP ANN method

In this subsection, the proposed MLP ANN is validated using experimental data of Nasrifar and Bolland (2006) study. The validations are performed for two different databases: pure methane and a Synthetic NG mixture. The temperature, pressure and JT coefficient as input

parameters input the network and the compressibility factor calculated then this Z-factor compared with Z-factor obtained from the study by (Nasrifar and Bolland, 2006). Table 2 shows the mole fraction of the Synthetic NG mixture that is used in the validation calculations (Nasrifar and Bolland, 2006).

Fig. 5 shows the error of compressibility factor calculation versus pressure on the constant temperature for pure methane and a Synthetic NG mixture. According to Fig. 5, the error percent of calculations for pure methane is between −1.5% and 1%. Also, the error percent of calculation for the Synthetic NG mixture is between −1% and 1%. Based on equation (26), the AAPD is 0.46% and 0.34% for pure methane and the Synthetic NG mixture, respectively.

The compressibility factor target obtained from (Nasrifar and Bolland, 2006) compared with the compressibility factor output that has been calculated using MLP ANN data is shown in Fig. 6. As seen in Fig. 6, the output and target data have good agreement with each other. Also, the R and RMSE of the calculations are 0.998 and 0.38%, respectively. The results obtained from the validations of the ANN MLP calculation indicate that the developed ANN could compute the compressibility factor with acceptable accuracy.

In the following step, the results of the proposed MLP ANN method have been compared to the GERG-2008 EOS results. Firstly, The JT coefficient and compressibility factor at various temperatures and pressure are calculated by utilizing GERG-2008 EOS. Then, the NG compressibility factor has been calculated by employing the proposed MLP ANN method. In this procedure, the temperature, pressure and JT coefficient are input parameters. Clearly, the compressibility factor calculated by the proposed ANN method should be the same as the compressibility factor calculated by GERG-2008 EOS. Table 3 shows the mole fraction (i.e. NG compositions) of natural gases that have been used for this purpose.

Fig. 7 represents the comparison of the calculated compressibility factor using the proposed ANN and the GERG-2008 EOS for two studied NG mixture (Khangiran and Bidboland). The compressibility factor plotted versus the JT coefficient and for the various constant temperatures. According to Fig. 7, for Khangiran composition, the proposed ANN method could predict the compressibility factor with high accuracy in all temperatures. For Bidboland compositions (As well as Kangan, Pars), the mentioned method could predict the compressibility factor with good accuracy except for low temperatures, for example in T = 250 K. Due to the low molecular weight of Khangiran NG (MW = 16.34), it could be concluded that, by decreasing the molecular weight of NG, the accuracy of the proposed ANN model increases.

Fig. 8 shows the error of compressibility factor calculation versus the JT coefficient in various constant temperatures for NG sources that are reported in Table 3. The results of Fig. 8 demonstrate that the error percent of the compressibility factor calculations, for all NG mixtures, are increased at low temperatures (close to the critical temperature). On the other hand, the natural gases with higher molecular weight are reported the more error percent to compute the compressibility factor.

Looking at Figs. 7 and 8, one could be realized that the developed method could predict the NG compressibility factor with acceptable accuracy for the temperature higher than T = 270 K. The accuracy of the model decreases as temperature approaches the critical temperature.

Fig. 9 represents the AAPD of NG compressibility factor calculations for various studied natural gases. According to Fig. 9, AAPD for the compressibility factor calculations is 0.385% for pure methane, 0.45% for Khangiran, 0.58% for Kangan, % 0.78 for Pars and is 1.12% for Bidboland.

3.2. Results of ANN MLP method

The output results of the proposed ANN MLP method as a polar plot is shown in Fig. 10. As seen, the compressibility factor plotted based on temperature, pressure and JT coefficient. Based on the information given in Fig. 10, if the deviation from the ideal gas state (i.e. Z-factor equal to one) at low temperatures (high pressures) is great, the value of the NG JT coefficient decreases. On the other hand, in the high temperatures (low pressure) the compressibility factor gets closer to one. In these conditions, the JT coefficient of NG increases. These types of graphs are very useful in the NG industry to obtain the compressibility factor without any knowledge of compositions.

4. Conclusion

In all EOS based methods for calculating the thermodynamic properties of the mixture (including NG compressibility factor), the mixture composition should be known for start. The compositions are usually measured through a costly process. Two widely accepted EOSs in NG industries are AGA8 and GERG-2008 which the latter is the most recent one. Employing these EOSs are very costly as measuring NG composition requires expensive devices.

The current study presents an intelligent approach for calculating NG thermodynamics properties without any knowledge of the composition. For this purpose, firstly, two NG thermodynamics properties (JT coefficient and compressibility factor) are computed for a wide range of temperature and pressure for 30,000 random datasets of compositions using GERG-2008 EOS. Based on these data sets of four thermodynamics properties, an ANN is developed in a way to compute NG compressibility factor while the other three properties are treated as input (pressure, temperature and JT coefficient). Due to the low cost of real-time measuring of these three properties, the current study presents a cost-effective method for real-time measuring of compressibility factor precisely.

The developed ANN method is validated with experimental data. The validations compared to experimental data are demonstrated that the statistical parameters include R, RMSE and AAPD are 0.998, 0.38% and 0.33%, respectively.

To show the accuracy of the developed approach, four different NG compositions are selected for evaluating purposes. The compressibility factor and JT coefficient are computed for various pressure and temperature range using the traditional approach.

Finally, the compressibility factor is determined using the intelligent approach when only pressure, temperature and JT coefficient are known. Then, the compressibility factor obtained from the ANN approaches is compared with the GERG-2008 results. The AAPD of NG compressibility factor calculations show 0.385% for pure methane, 0.45% for the Khangiran gas, 0.58% for the Kangan gas, 0.78% for the Pars gas and is 1.12% for the Bidboland gas. The results show that the overall AAPD is less than 0.7%, which indicates the high accuracy of the intelligent approach.

Credit author statement

Mahmood Farzaneh-Gord: Supervision, Conceptualization, Writing – review & editing. Hamid Reza Rahbari: Investigation, Validation, Writing – original draft. Behnam Mohseni-Gharesafa: Writing – original draft, Validation, Software, Investigation. Alexander Toikka: Investigation, Writing – original draft, Writing – review & editing. Irina Zvereva: Investigation, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

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