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Estimation of natural gas compressibility factors using artificial neural network approach

Ehsan Sanjari [a], Ebrahim Nemati Lay [a,b,*]

[a] Department of Chemical Engineering, Faculty of Engineering, University of Kashan, Ravand Street, Kashan, P.O. Box 87317-51167, Islamic Republic of Iran
[b] Energy Research Institute, University of Kashan, Kashan, Islamic Republic of Iran

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ABSTRACT

Prediction of compressibility factor of natural gas is an important key in many gas and petroleum engineering calculations. In this study compressibility factors of different compositions of natural gas are modeled by using an artificial neural network (ANN) based on back-propagation method. A reliable database including more than 5500 experimental data of compressibility factors is used for testing and training of ANN. The designed neural network can predict the natural gas compressibility factors using pseudo-reduced pressure and pseudo reduced temperature with average absolute relative deviation percent of 0.593. The accuracy of designed ANN has been compared to the mostly used empirical models as well as equations of state of Peng–Robinson and statistical association fluid theory. The comparison indicates that the proposed method provide more accurate results relative to other methods used in this work.

1. Introduction

Aside from crude oil and coal, natural gas is one of the most important primary energy sources accounting for almost one fourth of the world primary energy consumption due to its longer estimated future availability compared to crude oil (Statistical Review, 2006). Natural gas is a multi-component mixture of widely varying composition with methane as the main constituent and further essential components such as nitrogen, carbon dioxide, ethane, propane, and heavier hydrocarbons. Nowadays, natural gas is used for space heating, cooking, electric power generation, and as raw material in the chemical industry (Akansu et al., 2004). The accurate knowledge of the thermodynamic properties of natural gas and other mixtures of natural gas components is of indispensable importance for the basic engineering and performance of technical processes. This requires proper calculations for a wide range of mixture compositions and operating conditions in the homogeneous gas (Kunz et al., 2007). Through all thermodynamic properties of natural gas, the compressibility factor, which measures the deviations between real gas and ideal gas, is the most important parameter of gas engineering calculations. The rule of similar states shows that all natural gas mixtures with same reduced pressure and reduced temperature have approximately the same compressibility factor (Danesh, 1998). To calculate *z*-factor, equations of states (EOS), i.e., relationships between pressure, temperature, volume, and composition of matter, have been used widely in almost every branch of engineering, in particular for those industries dealing with gases. Empirical correlations and experimental data measurements are other common ways to estimate this parameter. Among all available methods for calculating natural gas compressibility factor, one of the most efficient and accurate method is artificial neural network (ANN). Neural networks are information-processing patterns based on the biological nervous systems, such as the brain, process information (Sivanandam et al., 2006). ANN has recently been used to predict pressure–volume–temperature (PVT) properties of pure gases by Moghadasi et al. (Moghadasi et al., 2009). Kamyab et al. have designed an ANN for estimating *z*-factor of natural gas mixture by using Katz diagram as input data (Kamyab et al., 2010) and Garrouch et al.

Abbreviations: AARD, average absolute relative deviation; ANN, artificial neural network; BP, back propagation; DA, Dranchuk–Abu-Kassem; EOS, equation of state; HMS, Heidaryan–Moghadasi–Salarabadi; HTP, Hankinson–Thomas–Philips; HY, Hall–Yarborough; LMA, Levenberg–Marguardt Algorithm; NG, natural gas; PCG, Pola–Ribiere Conjugate Gradient; PR, Peng–Robinson equation of state; RMSD, root mean square deviation; SCG, Scaled Conjugate Gradient.

* Corresponding author. Department of Chemical Engineering, Faculty of Engineering, University of Kashan, Ravand Street, Kashan, P.O. Box 87317-51167, Islamic Republic of Iran. Tel.: +98 361 5555 333; fax: +98 361 5559 930.
E-mail address: enemati@kashanu.ac.ir (E.N. Lay).

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considered application of ANN for estimating tight gas sands permeability (Garrouch and Samaui, 1996). Al-Quraishi et al. (AlQuraishi et al., 2011) have estimated the natural gas mixture density with an ANN by using 4445 experimental data with average absolute error of 4.93%. Also Al-Anazi et al. (Al-Anazi et al., 2011) predicted the compressibility factor of sour and natural gas by an artificial neural network system using 977 experimental data with average absolute percent of 0.965. On the other hands, equations of state are useful for description of fluid properties such as pressure–volume–temperature (PVT). However, the successful estimation of such correlations depends mainly on the range of data which have originated (Moghadasi et al., 2009). For equation of states, the binary interaction parameters should be adjusted using a reliable experimental data. Also empirical models are limited to range of operating conditions for predicting thermo-physical properties. Therefore, new models are highly required. The ANN's capability to estimate the PVT properties is one of the best estimating methods with high performance (Moghadasi et al., 2009). Few publications are available in literature for ANN applications in predicting *z*-factor of natural gas mixtures.

The main focus of this study is designing an appropriate ANN to estimate the *z*-factor of natural gas with higher accuracy than other ANN systems and models in desired temperature and pressure using more than 5500 experimental data (Seitz et al., 1996a, 1996b; Hou et al., 1996; Mihara et al., 1977; Douslin et al., 1964; Achtermann et al., 1992; Goodwin, 2009; Chuang et al., 1976; Schley et al., 2004; Younglove and Ely, 1987; Seitz and Blencoe, 1996; Fenghour et al., 1996; May et al., 2002; May et al., 2001; Sage and Lacey, 1939; Ababio et al., 2001; McElroy et al., 2001; Fenghour et al., 1999; Reamer et al., 1944; Capla et al., 2002; Patil et al., 2007; Zhou et al., 2006; Chamorro et al., 2006; Assael et al., 2001; Langelandsvik et al., 2007). Finally the results of the ANN model are compared to the mostly used empirical models and equations of state.

2. Natural gas compressibility factor

In the real gas equation, *z*-factor can be obtained as follow:

$$PV = ZnRT \tag{1}$$

Where P is pressure in kPa, V is the volume in liter, n is the number of gas mol, R is universal gas constant, T is temperature in K, and Z is the compressibility factor of gas.

The theory of corresponding states dictates that the *z*-factor can be uniquely defined as a function of reduced pressure and reduced temperature. The pseudo reduced pressure and temperature are defined by Eq. (2) and Eq. (3) respectively.

$$T_{pr} = T/T_{pc} \tag{2}$$

$$P_{pr} = P/P_{pc} \tag{3}$$

Where P_{pr} and T_{pr} are pseudo reduced pressure and temperature, respectively, T_{pc} is pseudo critical temperature and P_{pc} is pseudo critical pressure calculated as follows:

$$P_{pc} = \sum_{i=1}^{n} P_{ci} y_i \tag{4}$$

$$T_{pc} = \sum_{i=1}^{n} T_{ci} y_i \tag{5}$$

Where P_{ci} is critical pressure, T_{ci} is critical temperature, and y_i is the mole fraction of component i. By knowing of natural gas compositions, pseudo reduced pressure and pseudo reduced temperature, the compressibility factor of natural gas can be estimated by using empirical models. Some of the commonly used empirical correlations for calculation of *z*-factor are presented as follows:

2.1. Dranchuk and Abu-Kassem (DA) empirical method

In 1975 Dranchuk and Abu-Kassem proposed Eq. (6) with eleven-constant for calculating the gas compressibility factors (Dranchuk et al., 1975).

$$Z = \left[A_1 + \frac{A_2}{T_{pr}} + \frac{A_3}{T_{pr}^3} + \frac{A_4}{T_{pr}^4} + \frac{A_5}{T_{pr}^5}\right]\rho_r + \left[A_6 + \frac{A_7}{T_{pr}} + \frac{A_8}{T_{pr}^2}\right] \rho_r^2 - A_9\left[\frac{A_7}{T_{pr}} + \frac{A_8}{T_{pr}^2}\right]\rho_r^5 + A_{10}\left(1 + A_{11}\rho_r^2\right)\frac{\rho_r^2}{T_{pr}^3}\mathrm{EXP}\left[-A_{11}\rho_r^2\right] + 1 \tag{6}$$

Where ρ_r is reduced density of gas.

2.2. Heidaryan–Salarabadi–Moghadasi (HSM) empirical method

In 2010, Heidaryan et al. presented an accurate correlation for rapidly estimating of natural gas *z*-factor as Eq. (7) (Heidaryan et al., 2010):

$$Z = \frac{A_1 + A_2\ln\left(p_{pr}\right) + A_3\left(\ln p_{pr}\right)^2 + A_4\left(\ln p_{pr}\right)^3 + \frac{A_5}{T_{pr}} + \frac{A_6}{T_{pr}^2}}{1 + A_7\ln\left(p_{pr}\right) + A_8\left(\ln p_{pr}\right)^2 + \frac{A_9}{T_{pr}} + \frac{A_{10}}{T_{pr}^2}} \tag{7}$$

2.3. Peng–Robinson equation of state

The Peng–Robinson (PR) equation of state (EOS) is very effective for predicting *K*-values for hydrocarbon systems at medium to high pressures. Good results have been obtained by using this method for demethanizers, de-ethanizers, depropanizers, debutanizers and wellhead processes. The compressibility factors for both vapor and liquid phases can be calculated by using the PR equation of state. The PR EOS has been presented by Eq. (8) (Peng and Robinson, 1976):

$$p = \frac{RT}{V-b} - \frac{a}{V(V+b) - b(V-b)} \tag{8}$$

2.4. Statistical association fluid theory (SAFT) equation of state

The SAFT equation of state is similar to perturbed hard chain equations, but provides accuracy competitive with UNIQUAC, NRTL, or Wilson's equation for hydrogen bonding mixtures. The compressibility factor can be obtained from SAFT-EOS as Eq. (9) (Huang and Radosz, 1990):

$$Z = \frac{PV}{RT} = 1 + Z^{seg} + Z^{chain} + Z^{assoc} \tag{9}$$

3. Artificial neural network (ANN)

In order to find relationship between the input and output data derived from experimental works, a more powerful method than the traditional ones is necessary. ANN is an especially efficient algorithm to approximate any function with finite number of

discontinuities by learning the relationships between input and output vectors (Hagan et al., 1996). Neural networks have large degrees of freedom. Hence they are capable of modeling extremely complex functions by capturing the non-linearity of the process studied providing an efficient alternative to the traditional statistical methods (AlQuraishi et al., 2011). The structure of the information-processing system is constituted of an assemblage of several highly-interconnected elements of processing called neurons, working together to process the information and solve the problem. They are the result of scientific investigations that use mathematical formulations to model nervous system operations. The resulting techniques are being successfully applied in a variety of everyday technical, business, industrial, and medical applications (Sivanandam et al., 2006).

Fig. 1 shows multiple layers arrangement of a typical interconnected neural network which consist of an input layer, an output layer, and one hidden layer with different roles. Each connecting line has an associated weight.

Artificial neural networks are trained by adjusting the connection weights, so that the calculated outputs may be approximated by the desired values. The output from a given neuron is calculated by applying a transfer function to a weighted summation of its input to give an output, which can serve as input to other neurons, as follows (Gharbi, 1997):

$$\alpha_{jk} = F_k\left(\sum_{i=1}^{N_{k-1}} w_{ijk}\alpha_{i(k-1)} + \beta_{jk}\right) \tag{10}$$

Where α_{jk} are jth neuron outputs from kth layer and β_{jk} is the bias weight for neuron j in layer k. The model fitting parameters w_{ijk} are the connection weights. The nonlinear activation transfer functions F_k may have many different forms. The classical ones are threshold, sigmoid, Gaussian and linear function, etc. (Bulsari, 1995).

During training the weights and biases of the network are iteratively adjusted to minimize the network performance functions. One of typical performance function, used for training feed forward neural networks, is the network average absolute relative deviation percent (AARD %) that is presented in Eq. (11):

$$\text{AARD\%} = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{z_{i,\text{exp}} - z_{i,\text{calc}}}{z_{i,\text{exp}}}\right| \times 100 \tag{11}$$

Through different types of neural networks, the back propagation learning algorithm is the most commonly used algorithm to predict the properties of natural gases. Several back-propagations

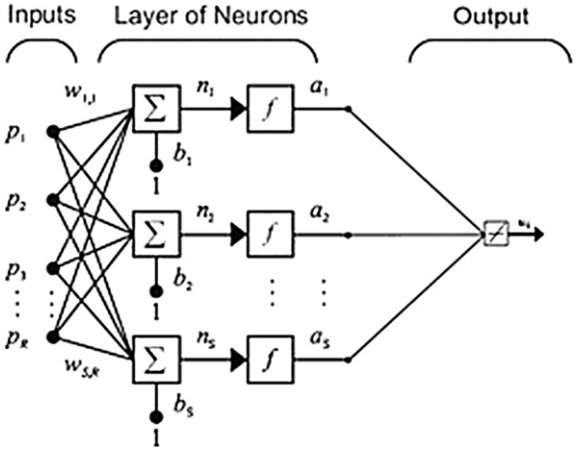

Fig. 1. The neural network structure.

Fig. 2. Determining the optimum number of neurons.

training methodologies exist, which include the Levenberg–Marguardt Algorithm (LMA), the Scaled Conjugate Gradient (SCG), the Pola–Ribiere Conjugate Gradient (PCG) and others. A review of investigations using similar applications indicates that the LMA is sufficiently robust and produces accurate ANNs (Eden and Inalli, 2009). The LMA, that is similar to Gauss–Newton method, is used in a back-propagation of error manner to reduce the average absolute relative deviation of the output.

The large collection of patterns needed to make a good quality ANN is commonly divided into three subsets, namely: training, validation, and test sets. The validation set is used to indicate the deviation produced during the training. This set is not used to alter the biases and weights, but serves to illustrate when the training should stop. Typically the deviation that was obtained with the set of validation should reduce during the training step, but should increase as the network starts to learn the specific training patterns used in the training set. The testing set is used to check the quality of the partitioning of the whole pattern set into these subsets. Thus, if the error in the testing set reaches a minimum value at

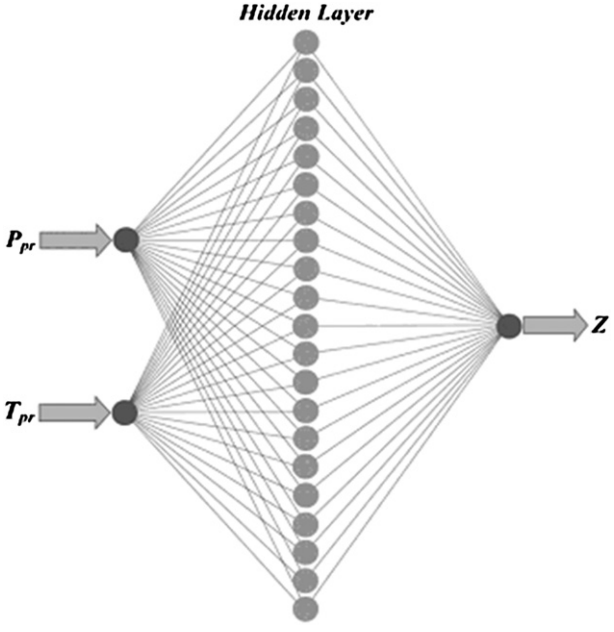

Fig. 3. Optimal back-propagation neural network paradigm.

Table 1
Average absolute relative deviation of this study compared to other empirical models and EOSs.

Methane (mole%)	Other component	Data points	*P* range (Mpa)	*T* range (K)	DA	HMS	PR	SAFT	ANN	Ref
0.5–0.9	CO_2	277	0.01–80	307–673	2.8762	5.1101	2.7114	0.9405	1.0864	(Seitz et al., 1996a; Seitz and Blencoe, 1996; Reamer et al., 1944)
0.5–0.9	N_2	455	0.6–80	240–673	1.6106	2.3193	2.1464	0.7913	0.8432	(Seitz et al., 1996a; Seitz and Blencoe, 1996; Ababio et al., 2001; Zhou et al., 2006)
0.6–0.8	CO_2–N_2	56	20–80	373–573	1.5438	1.4754	4.0402	0.6472	1.4354	(Seitz et al., 1996b)
0.54–0.94	H_2O	70	7.5–18.8	430–698	4.3349	5.377	0.3891	0.3565	1.3112	(Fenghour et al., 1996)
0.35–0.85	C_2	558	0.1–24.1	294–394	1.9081	5.0589	2.2584	0.9406	0.8344	(Hou et al., 1996; Sage and Lacey, 1939)
0.79–0.93	C_3	56	0.9–10	278–313	0.6971	3.9476	2.311	0.8687	0.9815	(May et al., 2002)
0.91–0.94	C_3–C_6	30	0.8–10.1	293–313	0.5511	5.5574	2.558	0.1939	0.8743	(May et al., 2001)
0.3–0.34	C_2–CO_2	60	0.7–7.5	283–333	3.0628	2.9833	2.4633	1.4118	0.9008	(Ababio et al., 2001)
0.35–0.53	C_4	71	8.8–48.1	316–479	1.5802	3.9886	1.487	0.6939	0.9321	(Fenghour et al., 1999)
0.55–0.81	H_2	109	0.4–51	273–348	1.4738	3.3327	1.8357505	0.6931	0.8854	(Mihara et al., 1977; Chuang et al., 1976)
1	–	3336	0.1–100	250–573	2.1609	2.5584	1.6887	0.5913	0.4312	(Seitz et al., 1996a; Hou et al., 1996; Mihara et al., 1977; Douslin et al., 1964; Achtermann et al., 1992; Goodwin, 2009; Chuang et al., 1976; Schley et al., 2004; Younglove and Ely, 1987)
0.8484	N.G.1	40	0.24–14	241–455	0.8099	11.3732	0.9832	0.1301	0.5832	(Assael et al., 2001)
0.9016	N.G.2	45	4.46–25.1	263–303	4.0135	11.6532	1.1834	0.8112	0.4936	(Langelandsvik et al., 2007)
0.8001	N.G.3	34	13.3–25.3	262–304	13.2343	17.8473	4.4563	1.6011	1.0323	(Langelandsvik et al., 2007)
0.922	N.G.4	45	4.9–25.2	262–304	4.0129	7.0848	3.0021	0.7353	0.2122	(Langelandsvik et al., 2007)
0.8957	N.G.5	224	0.1–20.1	260–320	3.5317	8.2178	3.6513	0.9919	0.7234	(Schley et al., 2004)
0.8433	N.G.6	224	0.1–20.2	269–320	2.6531	8.7632	1.9734	1.1032	0.3144	(Schley et al., 2004)
0.9835	N.G.7	28	1.0–15	253–323	0.9843	1.8322	0.8812	0.4512	0.738	(Capla et al., 2002)
0.9036	N.G.8	28	1.0–15	253–323	0.7916	2.0003	0.8113	0.5087	0.3239	(Capla et al., 2002)
0.9244	N.G.9	28	1.0–15	253–323	1.1569	3.1456	1.7632	0.4257	0.9324	(Capla et al., 2002)
0.9099	N.G.10	70	2.2–34.5	263–350	3.4362	3.8321	2.3421	0.9588	0.4448	(Zhou et al., 2006; Chamorro et al., 2006)
Average		**5844**			**2.2684**	**3.7086**	**1.9566**	**0.7097**	**0.5935**	

a significantly various iteration number of that in which the minimum occurs with the validation set, this might indicate a poor division of the original data set.

A set of data containing pseudo reduced pressure, pseudo reduced temperature and compressibility factor was collected from experimental data. The database contains more than 5500 points of natural gas compressibility factors reported in the literature (Seitz et al., 1996a, 1996b; Hou et al., 1996; Mihara et al., 1977; Douslin et al., 1964; Achtermann et al., 1992; Goodwin, 2009; Chuang et al., 1976; Schley et al., 2004; Younglove and Ely, 1987; Seitz and Blencoe, 1996; Fenghour et al., 1996; May et al., 2002; May et al., 2001; Sage and Lacey, 1939; Ababio et al., 2001; McElroy et al., 2001; Fenghour et al., 1999; Reamer et al., 1944; Capla et al., 2002; Patil et al., 2007; Zhou et al., 2006; Chamorro et al., 2006; Assael et al., 2001; Langelandsvik et al., 2007). The natural gas mixtures have different molecular weights from 11.3 to 30.

Neural network training can be made more efficient if certain preprocessing steps are performed on the network inputs and targets. The neurons in the hidden layer perform two tasks: summing the weighted inputs connected to them and passing the result through a nonlinear activation function to the output or adjacent neurons of the corresponding hidden layer. By using LM algorithm that is more accurate than other back-propagation methods, more than 70% of data set is used to train each ANN

Table 2
Compositions of 10 different natural gas mixtures mentioned in Table 1.

	N.G.1	N.G.2	N.G.3	N.G.4	N.G.5	N.G.6	N.G.7	N.G.8	N.G.9	N.G.10
Methane	84.84	90.16	80.0079	92.2045	89.57	84.33	98.352	90.362	92.436	90.991
Ethane	8.4	6.3077	9.3063	4.3373	6.1464	3.4085	0.511	5.708	1.285	2.949
Propane	0.5	0.801	4.963	0.5396	1.2532	0.6023	0.153	1.124	0.348	1.513
n-Butane	–	0.0643	1.2791	0.0771	0.1924	0.1282	0.031	0.169	0.046	0.755
i -Butane	–	0.0446	0.7188	0.2562	0.2857	0.1033	0.021	0.301	0.041	0.755
n-Pentane	–	0.0044	0.2499	0.0198	0.0324	0.035	0.011	0.029	0.014	0.304
i -Pentane	–	0.0054	0.2556	0.0468	0.0565	0.0375	0.008	0.059	0.015	0.299
Hexane	–	0.0014	0.1793	0.0606	0.0572	0.0388	0.005	0.058	0.012	–
Heptane	–	0.0005	0.101	0.0364	0.034	0.0174	0.001	0.035	–	–
Heptane+	–	0.0001	0.0621	0.0091	0.0095	0.0072	0.0003	0.008	–	–
Hydrogen	–	–	0.001	0.0005	0.0007	0.0005	–	–	–	–
Helium	–	0.0068	0.0084	0.0168	0.0137	0.052	–	0.015	–	–
Water		0.0006	–	–	–	–	–	–	–	–
Argon	–	0.0514	–	–	0.0419	0.01	–	0.011	–	–
Nitrogen	5.6	0.7587	0.6601	1.3916	1.5324	9.752	0.841	1.474	5.751	2.031
Carbon dioxide	0.66	1.7947	2.1902	1.003	0.774	1.4523	0.066	0.647	0.052	0.403
Benzene	–	0.0002	0.0173	0.0007	–	0.025	–	–	–	–

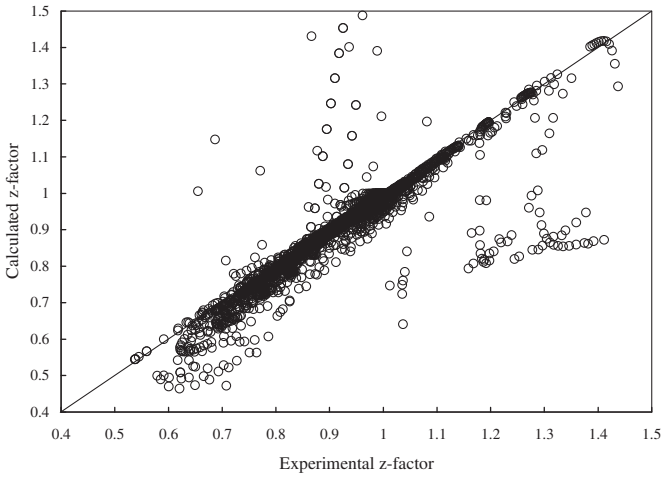

Fig. 4. A comparison between Dranchuk–Abu-Kassem (DA) empirical model and experimental data.

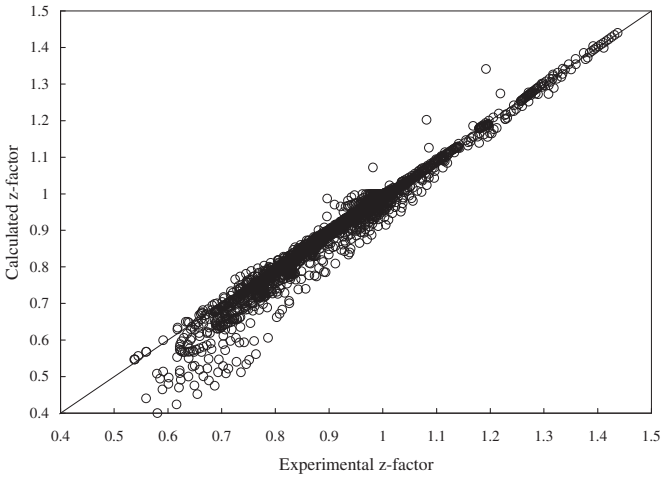

Fig. 6. A comparison between Peng–Robinson EOS (PR) and experimental data.

and the rest have been used to evaluate their accuracy and trend stability using LM algorithm. Number of hidden neurons has been systematically varied to obtain a good estimate of the trained data. To find the optimum number of nodes in the hidden layer, which provides good estimates of the output, different number of neurons was considered. The criterion for selection was AARD% between network output and training data. The results are illustrated in Fig. 2. As shown in Fig. 2, architecture of ANN having 21 neurons gave the least average relative error for the training data set with AARD% of 0.593. Fig. 3 shows the network architecture with 21 neurons in hidden layer.

4. Result and discussion

The results showed the accuracy of designed ANN for estimating natural gas *z*-factors. Table 1 reports the average absolute relative deviation percent (AARD%) of ANN compared to the commonly used empirical models and equations of state for different natural gas mixtures. Where, the compositions of natural gas namely "N.G.1" to "N.G.10" are listed in Table 2.

Figs. 4–7 show the comparison of the experimental data versus empirically derived correlations of DK and HSM as well as Peng–Robinson and SAFT equations of state, respectively. Fig. 8 shows the comparison of the experimental data versus the computed neural network data. It can be seen from Table 1 that the designed ANN model can predict *z*-factors better than the commonly used empirical models and equations of state. Fig. 9 shows the cumulative frequency of obtained network versus AARD% of method compared to all other models. It shows the accuracy of presented method in estimation of compressibility of more than 5500 measurements as compared to other methods discussed in this study. The new method has successfully predicted 74% of the all measurements with AARD% of less than 0.5, and 84% of the data with AARD% of less than 1. Only 5% of the compressibility measurements were predicted with AARD% on the order of 3–10% by the new method. SAFT, which is the second accurate method, predicted 56% of the *z*-factor measurements with AARD% of less than 0.5, and 78% of the data with AARD% of less than 1%. Hence the neural network advantage over all the methods was considered in this study. To estimate the applicability of artificial neural network approach for calculation of compressibility factor of various natural gases, the experimental data and computed data from ANN and other mentioned empirical correlations for *z*-factor versus pseudo reduced pressure at constant temperature for three different natural gas mixtures are presented in Figs. 10–13. NG1 contains 33.24% CH_4, 32.07% C_2H_6 and 34.69% CO_2 (McElroy et al.,

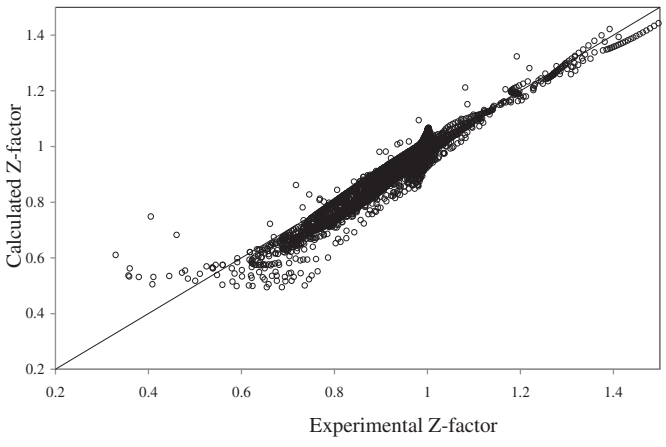

Fig. 5. A comparison between Heydarian et al. (HMS) empirical model and experimental data.

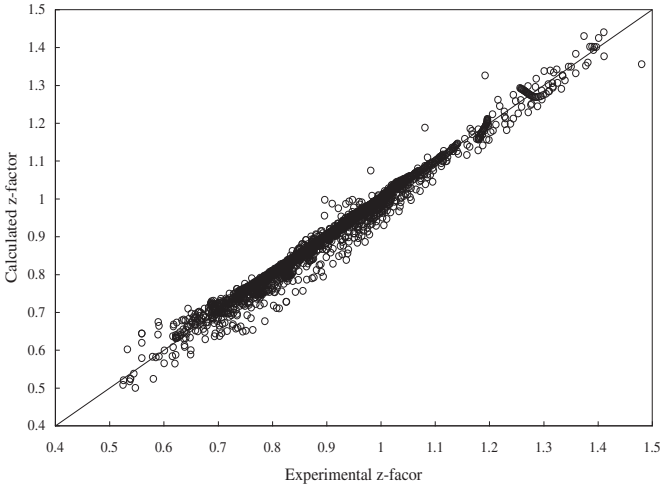

Fig. 7. A comparison between SAFT-EOS and experimental data.

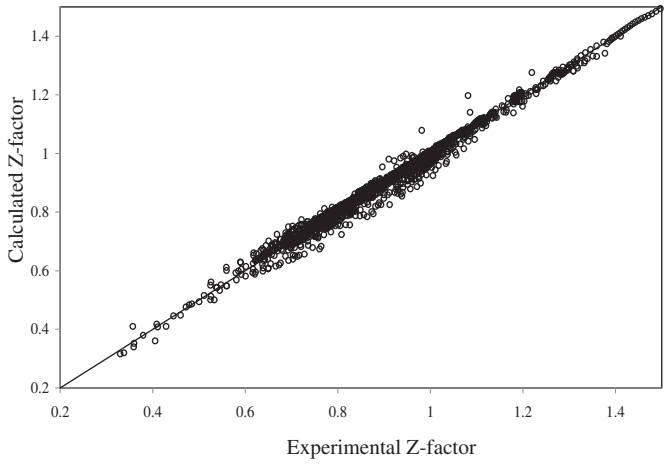

Fig. 8. A comparison between ANN and experimental data.

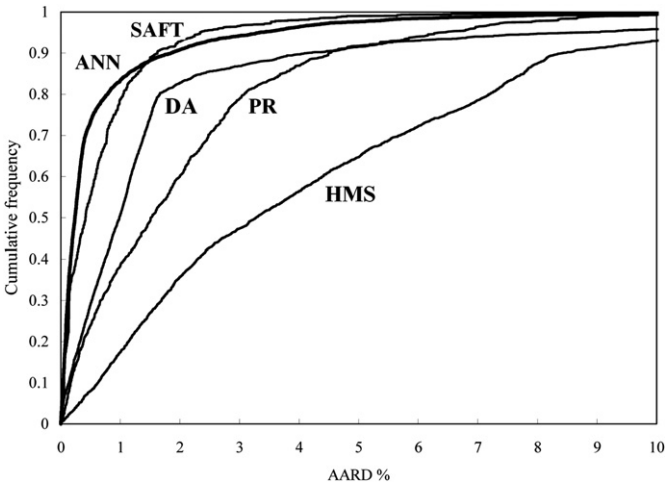

Fig. 9. Cumulative frequency as a function of AARD%.

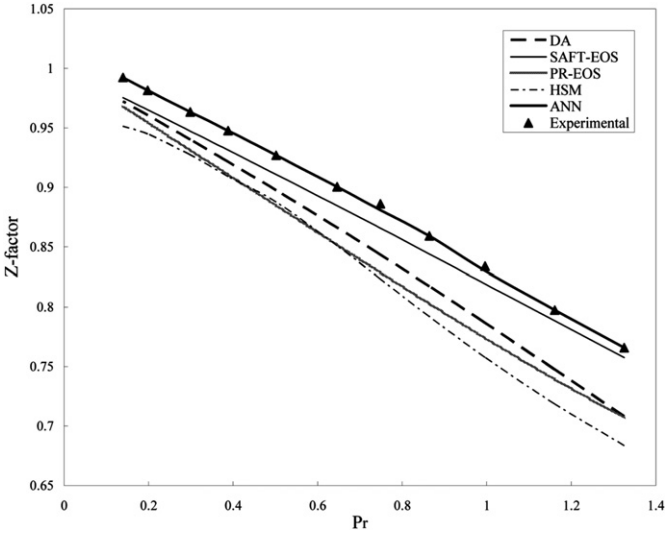

Fig. 10. Experimental data and results of ANN and other method for mixture1 ($CH_4 = 33.24\%$).

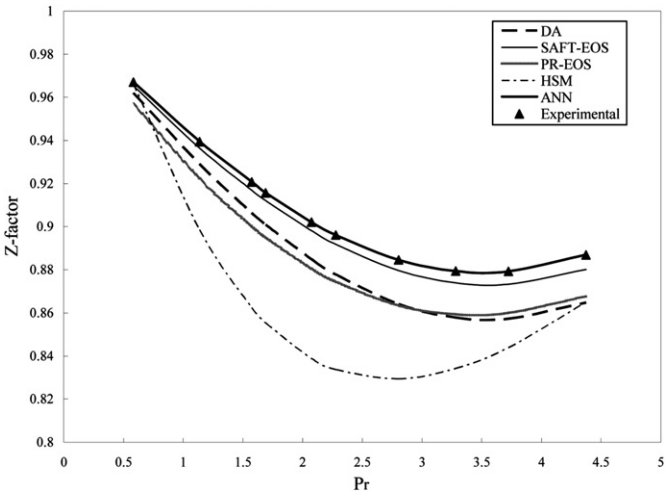

Fig. 11. Experimental data and results of ANN and other method for mixture2 ($CH_4 = 80\%$).

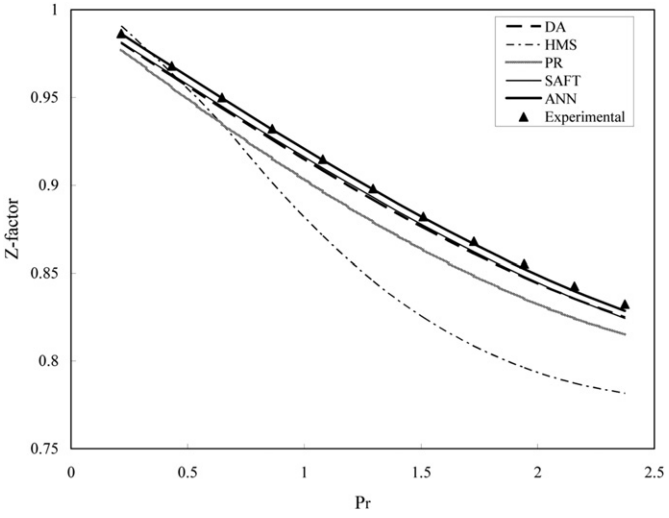

Fig. 12. Experimental data and results of ANN and other method for mixture3 ($CH_4 = 98.64\%$).

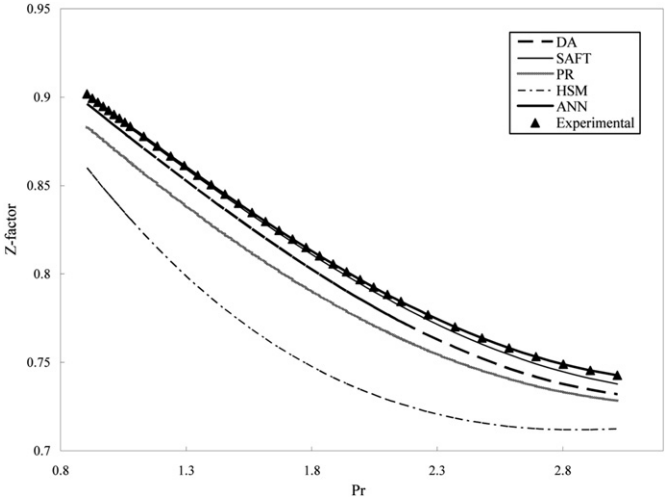

Fig. 13. Experimental data and results of ANN and other method for mixture4 ($CH_4 = 100\%$).

2001). "NG2" contains 80% CH_4 and 20% N_2 (McElroy et al., 2001), "NG3" contains 98.64% CH_4 and 0.6% C_2H_6 (Farzanehgard et al., 2008), and "NG4" is pure methane (Achtermann et al., 1992). As shown in Figs. 10–13, the designed ANN is much more accurate than other methods for prediction of compressibility factors.

5. Conclusion

In this study, the compressibility factors of different compositions of natural gas are modeled by using an artificial neural network (ANN) based on LMA algorithm back-propagation method. A reliable database of compressibility factors for testing and training of ANN has been used. The results of the ANN model are compared to the empirical models of DK and HSM as well as equations state of PR and SAFT. The comparison showed that the designed ANN model can predict *z*-factors of natural gas mixtures more accurately than other methods studied here.

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Nomenclature

ρ_r: reduced density
T_{pr}: pseudo reduced temperature
P_{pr}: pseudo reduced pressure
P_{pc}: pseudo critical pressure
T_{pc}: pseudo critical temperature
Z: compressibility factor
n: mole number
R: universal gas constant
T: temperature
P: pressure
A: constant parameter
a: equation of state energy parameter
b: equation of state volume parameter
α: neuron number
β: bias weight
w: connection weight
F_k: nonlinear activation transfer function
assoc: association
calc: calculation
exp: experimental
seg: segment