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Novel natural gas molecular weight calculator equation as a functional of only temperature, pressure and sound speed





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ABSTRACT

In city gate stations (CGS) experimental facilities are currently employed to specify natural gas compositions and subsequently calculate its density. Then, natural gas mass flow rate is calculated by employing an Ultrasonic Flow Meter (UFM), and a volume corrector to convert the given value to its equivalent in standard conditions. As online measurement of natural gas compositions is a costly and difficult task, this study presents an innovative method for natural gas mass flow metering in CGSs. In this method, a novel correlation, which is a functional of only three simple measurable variables i.e. temperature, pressure and sound speed, is presented for calculating natural gas molecular weight, and then, employing the authentic equations of state (EOS) of AGA8 for natural gas, its density could be calculated. The correlation was developed based on curve fitting and data mining approaches on a large database associated with four different natural gas fields of Iran and its accuracy was validated with available experimental data for seven other Iran's natural gas fields and two more gases with sample compositions. Each database in correlation development and validation stage (13 databases altogether) consists of 17,000 sound speed values in all possible temperature and pressure ranges in CGSs after expansion process. Mean absolute error (MAE) and mean absolute percentage error (MAPE) methods are used to validate the correlation accuracy and compare its performance with the correlation presented previously for the same objective. The evaluation results prove high prediction accuracy for the presented correlation and its superiority comparing to the previous work.

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1. Introduction

Natural gas mass flow metering is a big problem in natural gas distribution systems as its compositions, even in an individual natural gas pipeline, could vary significantly over time. Therefore, sophisticated experimental facilities are required to measure the natural gas compositions and removing these facilities from mass flow metering systems in transmission pipelines (specially CGSs) has been the concern of experts working in this area. Over the last years, many devices such as multiple ultrasonic transient-time meters as alternative devices for conventional orifice plates and turbine meters have been employed for natural gas metering (Froysa and Lunde, 2005). Basically, these devices meter the stream volume flow rate and the natural gas density is also required for

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calculating its mass flow rate. Natural gas density can be directly measured, independent of pressure and temperature effects, by Coriolis density meters; mass flow controllers; gas chromatographs and etc. However, there are some disadvantages with such devices and their most highlighted disadvantage is that the use of these devices is work demanding and costly. Also, another aspect of importance in these instruments is the ability of detecting drift as a common problem. That's why; reducing the number of such devices in metering stations (specifically CGS) is highly addressed in the corresponding studies (Smalling et al., 1986; Valdes and Cadet, 1991).

For this aim, many studies have already been done and the number of studies in this area is increasing so fast. For example, Ref. (Smalling et al., 1986) refers to an invention that introduces an apparatus for flow metering in tubes. However, this apparatus is only suitable for low concentration gases and in the velocity range of 0-50 ft/s and even in this velocity range, prediction deviations up to 2% is expected for mass flow metering. Therefore, this is clear

that the device could not be recommended to be used in CGSs as not only natural gas is not a low concentration composition, but also in a CGS, in many cases, the velocity of natural gas stream is higher than 50 ft/s. Also, 2% prediction deviation for mass flow rate seems to be much more than standard levels. Ref. (Hiismaeki, 1993) also points out to another device made for the same objective: however, this instrument is only applicable for such low pressures in which natural gas behaves like an ideal gas while natural gas status through CGSs is far away from an ideal gas. Ref. (Valdes and Cadet, 1991) employs the heavy virial equation (Hirschfelder et al., 1964) to calculate natural gas molecular weight based on the computed sound speed as a functional of pressure, temperature and gas compositions. Although the device accuracy is really high, the compositions of the natural gas mixture are still required in this method. There are other similar works which are worth mentioning in this area (Hammond, 2001; Watson and A White, 1982; Dell'Isola et al., 1997; Buonanno et al., 1998).

On the other hand, EOSs are widely used for computing natural gas density. Most broadly employed standard EOSs for natural gas are AGA8 and GERG2008 (AGA8 and Compressibility and, 1992; Farzaneh-Gord and Rahbari, 2011). However, even these EOSs, in addition to temperature and pressure, need either the natural gas compositions or molecular weight, for calculating its density. In fact, knowing the compositions, these EOSs calculate the natural gas molecular weight and subsequently, this value is used for density measurement (Farzaneh-Gord and Rahbari, 2011). Therefore, what is the main essential information of these EOSs for density metering is the mixture molecular weight. It is worth mentioning that AGA8 and GERG2008 are not the only equations that could be used for density measurement of natural gas mixtures and several more correlations have been developed for this objective. Dranchuk and Abou-Kassem developed a gas density calculator correlation utilizing 1500 data points, including pure gases and gas mixtures from different sources (Dranchuk and Abou-Kassem, 1975). Londono et al. reported simplified correlations for calculating the density of hydrocarbon gases like natural gas (Londono et al., 2002). Al-Quraishia and Shokirb employed Alternating Conditional Expectations (ACE) algorithm and presented a new equation for computing the density of hydrocarbon gases and pure and impure gas mixtures (AlQuraishi and Shokir, 2009). There are also other authentic references in this field (Gysling, 2007; Hall and Holste, 1995; Farzaneh-Gord et al., 2015c; Standing and Katz, 1942; Weberg, 1990). In another work, Farzaneh-Gord and Rahbari developed novel correlations for calculating most thermodynamic and thermal properties of natural gas such as density based on AGA8 EOS (Farzaneh-Gord and Rahbari, 2011). In the mentioned study, each thermodynamic property is a functional of natural gas pressure, temperature and specific gravity. These methods were developed by Farzaneh-Gord and Rahbari (Farzaneh-Gord and Rahbari, 2011) and were previously presented in Farzaneh-Gord et al. (Farzaneh-Gord et al., 2010; Farzaneh-Gord and Rahbari, 2012) and Marić (Marić, 2005, 2006; Marić et al., 2004).

Also, in one of the last studies in this area, Farzaneh-Gord et al. (Farzaneh-Gord et al., 2015a) developed a correlation to calculate natural gas molecular weight as a functional of temperature, pressure and Joule—Thomson coefficient of natural gas in CGSs. In an almost similar manner, this works presents a novel correlation for calculating the molecular weight of natural gas stream just as a functional of its pressure, temperature and sound speed while there is no information about its compositions. Having the value of molecular weight calculated by the presented correlation, one could then calculate the natural gas density by employing AGA8 EOS. Finally, using the value of density given by AGA8 EOS and the data given by the UFM and volume corrector existent at the CGS,

natural gas mass flow rate passing through the CGS is easily calculated. The main advantage of the current study relative to Ref. (Farzaneh-Gord et al., 2015a) is that the accuracy of the correlation presented in this work almost doubles. Also, in contrast with the previous study in which CGS configuration needed to be revised by adding some facilities to measure natural gas Joule—Thomson coefficient, the CGS conventional configuration is not supposed to be amended in this method. Detailed information related to the proposed approach is presented in sections 3 and 4. It should be mentioned that the correlation development and its validation has been done by accurate curve fitting and data mining method on a large database associated with 11 major natural gas fields of Iran and two more sample gases.

2. Current flow metering method

The first question may arise here is that what a CGS is. In fact, a CGS is a station close to natural gas consumption points in which natural gas pressure is reduced significantly, from almost 1000 psi to 250 psi (Farzaneh-Gord et al., 2011; Farzaneh-Gord et al., 2012; Arabkoohsar et al., 2015; Farzaneh-Gord et al., 2015; Arabkoohsar et al., 2014). As it was mentioned before, CGS is one of main places in natural gas transmission system in which mass flow metering is carried out. Fig. 1 illustrates how natural gas mass flow rate is currently measured in CGSs of Iran (and probably other countries as well). According to the figure, experimental facilities are employed to measure natural gas compositions, and subsequently its density. Also, in addition to temperature and pressure gauges, there is a UFM to calculate the natural gas stream velocity. Finally, a volume corrector receives all these four measured values (i.e. natural gas stream velocity, its temperature, pressure and density) to calculate the natural gas mass flow rate based on standard condition $(P = 0.1 \text{ MPa and } T = 25 \circ C).$

The main problem of this method is the high deviation of gas density relative to the actual value as it is measured once or at most twice a year because natural gas composition measurement process by the experimental facilities is really costly. Therefore, as long as the experimental instruments or online density meter instruments are available, natural gas density could be calculated accurately; otherwise, mass flow rate measurement would not be accurate enough. That's why presenting novel, simple and accurate real time methods of natural gas mass flow metering seems to be very beneficial.

3. The proposed idea

Based on the presented information in introduction section, the main goal of this work is to facilitate natural gas mass flow metering in CGSs as one main places of natural gas industry. For this objective, a novel correlation for molecular weight calculation of natural gas mixtures just as a functional of three easy measurable parameters, i.e. natural gas temperature, pressure and sound speed, is developed. Then, using the calculated value of molecular weight by this correlation along with the natural gas temperature and pressure as the essential input information of AGA8 EOS (as one of



Fig. 1. Natural gas mass flow rate metering process diagram.

the most reliable EOSs for natural gas), natural gas density could be calculated. Therefore, in this approach, no information about natural gas compositions is required and density measurement experimental facilities could be removed from the configuration of mass flow metering unit of CGSs shown in Fig. 1. Clearly, real time measuring of natural gas stream pressure and temperature could be carried out by simple sensors. However, the question may arise here is how to measure natural gas sound speed. In fact, this is the positive point of the proposed measurement method in this work as UFMs, in addition to volume flow metering, are able to measure sound speed (Dadashnialehi and Moshiri, 2011). As a results, in contrast with the previous study (Farzaneh-Gord et al., 2015a) in which adding Joule-Thomson coefficient calculator facilities to the CGS was needed, no change in flow metering unit of CGS will happen in this method. Fig. 2 shows the schematic diagram of the proposed system.

According to the figure, a very simple processor which employs the presented correlation to estimate the idiomatic molecular weight as well as AGA8 EOS subsequently for calculating the density has been added to the conventional mass flow measurement configuration and the density metering facilities have totally been removed. Also, in this configuration, the UFM measures both sound speed (as an essential information of molecular weight calculator equation) and natural gas stream velocity for the volume corrector.

Ultrasonic transit time flow meters measure the time of ultrasonic pulses propagating in and against the direction of flow as t_{up} and t_{down} . Having these values as well as the distance between transducers and the inclination angle (ϕ), one could calculate the average flow velocity (V) and sound speed (C) by Equations (1) and (2), respectively. Fig. 3 illustrates an ultrasonic transit time flow meter schematic (Hans and Windorfer, 2003; Bo and Li, 2013; Tezuka et al., 2008).

$$V = \frac{L}{2\sin\varphi} \frac{t_{up} - t_{down}}{t_{up} t_{down}}$$
(1)

$$C = \frac{L}{2} \frac{t_{up} + t_{down}}{t_{up} t_{down}}$$
(2)

As it was explained, this work aims at presenting a molecular weight calculator equation which is a functional of temperature, pressure and sound speed. At first sight, it may seem impossible to calculate molecular weight as a functional of some parameters such as temperature and pressure, because molecular weight changes by variation of neither temperature nor pressure and the only parameter which affects molecular weight value is the mixture compositions.

$$MW = f(compositions)$$
(3)



Fig. 2. The schematic diagram of the proposed system for natural gas mass flow metering in CGSs; T: temperature, P: pressure, C: sound speed, V: velocity.



Fig. 3. The schematic diagram of an ultrasonic transit time flow meter.

However, the estimated value by the correlation operates as an idiomatic molecular weight which changes by variation of temperature, pressure and sound speed as:

$$MW_{id} = f(T, P, C) \tag{4}$$

Where T, P and C refer to temperature, pressure and sound speed in the natural gas stream, respectively. By employing this idiomatic molecular weight, natural gas density could be calculated by AGA8 EOS as follow (Dranchuk and Abou-Kassem, 1975):

$$\rho = f(T, P, MW_{id}) \tag{5}$$

Having this value, one could easily calculate natural gas mass flow rate as below:

$$\dot{\mathbf{m}} = \rho \mathbf{V} \mathbf{A}$$
 (6)

Where ρ , V and A refer to density, velocity and sectional area of the pipe, respectively.

4. The new developed correlation

In this section, the correlation development process is comprehensively described. As it was claimed before, the correlation is supposed to be developed based on curve fitting and data mining approaches. Therefore, one needs an actual and reliable database for this objective. The database employed in this work includes sound speed values in all possible temperatures and pressure ranges after expansion process in CGSs for 11 major natural gas fields of Iran and two sample gases. Table 1 details the compositions of the 11 natural gas fields of Iran. It is worth mentioning that the first four mixtures were used to develop the correlation and the other fields have been used to verify the accuracy of the correlation. It also bears mentioning that Gasho is a sour gas among the considered fields in correlation development procedure and it was considered intentionally to make the correlation applicable for even sour gases and, on the other hand, Bidboland, as another sour gas, was considered in validation procedure to evaluate the correlation accuracy for such sour natural gases.

The information related to these natural gas mixtures compositions was provided by National Iranian Gas Company (NIGC), Semnan division (iraniangas). Then, for producing the required database, employing these mixtures compositions as well as different temperature and pressure values as the essential input information of AGA8 EOS, the value of sound speed in different temperatures and pressures for each natural gas mixture was calculated. As a result, in the end, an extensive database including 17,000 sound speed values for each natural gas field in different temperatures and pressures was produced.

Table 1
The compositions and actual molecular weight of different natural gas fields in Iran.

	Torkman	Kangan	Shurjeh	Gasho	Khangiran	Qeshm	Aghar	Gonbadly	Sarkhoon	Pars	Bidboland
CH4	94.21	90.04	90.04	79.08	98.6	87.79	90.31	88.05	92.39	87	80.01
C2H6	2.25	3.69	3.69	0.91	0.59	1.55	1.45	1.4	3.63	5.4	1.38
C3H8	0.53	0.93	0.93	0.36	0.09	0.87	0.43	0.34	1.49	1.7	0.49
I-C4H10	0.36	0.2	0.2	0.09	0.02	0.24	0.11	0.09	0.39	0.3	0.34
N-C4H10	0	0.29	0.29	0.18	0.04	0.47	0.17	0.13	0.51	0.45	0.65
I-C5H12	0.26	0.14	0.14	0.08	0.02	0.22	0.08	0.07	0.25	0.13	0.10
N-C5H12	0	0.08	0.08	0.07	0.02	0.2	0.06	0.06	0.26	0.11	0.09
N-C6H14	0.17	0.14	0.14	0.69	0.07	0.47	0.14	0.03	0.27	0.07	0.09
+C7H16	0.18	0.01	0.01	0	0	0	0.15	0.33	0	0.03	0
N2	1.9	4.48	4.48	5.14	0.55	8.14	5.58	7.85	0.81	3.1	5.41
CO2	0.14	0	0	7.08	0	0.05	1.4	1.63	0	1.71	8.41
H2S	0	0	0	6.32	0	0	0.007	0	0	0	3.03
H20	0	0	0	0	0	0	0.113	0.02	0	0	0
MW(kg/kmol)	18.66	17.79	17.71	20.67	16.36	18.36	17.85	18.17	17.58	18.69	20.51

Having this database, now one could proceed to develop the idiomatic molecular weight calculator equation as a functional of temperature, pressure and sound speed. For this objective, as the first step of formulation, idiomatic molecular weight should be defined as a functional of the gas mixture sound speed. For this aim, an accurate curve fitting is done on sound speed values for different natural gas mixtures with their own molecular weights in specific temperatures and specific pressures. The curve fitting results show that natural gas idiomatic molecular weight varies as a quadratic function of its sound speed as below:

$$MW_{id} = XC^2 + YC + Z \tag{7}$$

Where, C refers to the mixture sound speed and X, Y and Z are constant coefficients of the correlation for different temperatures and pressures. The second step of formulation is, then, determining the idiomatic molecular weight of the mixture variation versus its pressure for which the constant coefficients in the above equation should be found as a functional of pressure. Doing another curve fitting on different values of X, Y and Z in different pressures reveals that a quadratic function of pressure for each of the constant coefficients could make an exact estimation for idiomatic molecular weight variation versus pressure. Thus, the constant coefficients in Equation (7) should be as below:

$$X = X_2 P^2 + X_1 P + X_0$$

$$Y = Y_2 P^2 + Y_1 P + Y_0$$

$$Z = Z_2 P^2 + Z_1 P + Z_0$$
(8)

Where P refers to the mixture pressure and X_2 , X_1 , X_0 , Y_2 , Y_1 , Y_0 and Z_2 , Z_1 , Z_0 are constant coefficients for different temperatures. Considering these constants, Equation (7) could be re-written as follow:

$$\begin{split} \mathsf{MW}_{id} &= \left(X_2 \mathsf{P}^2 + X_1 \mathsf{P} + X_0 \right) \mathsf{C}^2 + \left(Y_2 \mathsf{P}^2 + Y_1 \mathsf{P} + Y_0 \right) \mathsf{C} + \left(Z_2 \mathsf{P}^2 \right. \\ &+ Z_1 \mathsf{P} + Z_0 \Big) \end{split}$$

By far, the idiomatic molecular weight of natural gas mixture can be calculated at a specific temperature. Therefore, the only remaining step is finding how this item varies by temperature changes. Finally, as the last step of the formulation, while there are nine constant coefficients in each specific temperature, the third curve fitting should be done on these constant coefficients and temperature values to reveal the idiomatic molecular weight dependency on temperature. However, this time, a cubic time dependent function found to be much more accurate than a quadratic function. Thus, the nine constant coefficients in the above equation could be re-written as below:

$$\begin{split} X_{2} &= X_{23}T^{3} + X_{22}T^{2} + X_{21}T + X_{20} \\ X_{1} &= X_{13}T^{3} + X_{12}T^{2} + X_{11}T + X_{10} \\ X_{0} &= X_{03}T^{3} + X_{02}T^{2} + X_{01}T + X_{00} \\ Y_{2} &= Y_{23}T^{3} + Y_{22}T^{2} + Y_{21}T + Y_{20} \\ Y_{1} &= Y_{13}T^{3} + Y_{12}T^{2} + Y_{11}T + Y_{10} \\ Y_{0} &= Y_{03}T^{3} + Y_{02}T^{2} + Y_{01}T + Y_{00} \\ Z_{2} &= Z_{23}T^{3} + Z_{22}T^{2} + Z_{21}T + Z_{20} \\ Z_{1} &= Z_{13}T^{3} + Z_{12}T^{2} + Z_{11}T + Z_{10} \\ Z_{0} &= Z_{03}T^{3} + Z_{02}T^{2} + Z_{01}T + Z_{00} \end{split}$$
(10)

Finally, taking Equations (7)–(10), one could write the final format of natural gas idiomatic molecular weight calculator, developed just as a functional of its temperature, pressure and sound speed, as:

$$\begin{split} \mathsf{MW}_{id} &= \left[\left(\mathsf{X}_{23}\mathsf{T}^3 + \mathsf{X}_{22}\mathsf{T}^2 + \mathsf{X}_{21}\mathsf{T} + \mathsf{X}_{20} \right) \mathsf{P}^2 + \left(\mathsf{X}_{13}\mathsf{T}^3 + \mathsf{X}_{12}\mathsf{T}^2 \right. \\ &\quad + \mathsf{X}_{11}\mathsf{T} + \mathsf{X}_{10} \right) \mathsf{P} + \left(\mathsf{X}_{03}\mathsf{T}^3 + \mathsf{X}_{02}\mathsf{T}^2 + \mathsf{X}_{01}\mathsf{T} + \mathsf{X}_{00} \right) \right] \mathsf{C}^2 \\ &\quad + \left[\left(\mathsf{Y}_{23}\mathsf{T}^3 + \mathsf{Y}_{22}\mathsf{T}^2 + \mathsf{Y}_{21}\mathsf{T} + \mathsf{Y}_{20} \right) \mathsf{P}^2 + \left(\mathsf{Y}_{13}\mathsf{T}^3 + \mathsf{Y}_{12}\mathsf{T}^2 \right. \\ &\quad + \mathsf{Y}_{11}\mathsf{T} + \mathsf{Y}_{10} \right) \mathsf{P} + \left(\mathsf{Y}_{03}\mathsf{T}^3 + \mathsf{Y}_{02}\mathsf{T}^2 + \mathsf{Y}_{01}\mathsf{T} + \mathsf{Y}_{00} \right) \right] \mathsf{C} \\ &\quad + \left[\left(\mathsf{Z}_{23}\mathsf{T}^3 + \mathsf{Z}_{22}\mathsf{T}^2 + \mathsf{Z}_{21}\mathsf{T} + \mathsf{Z}_{20} \right) \mathsf{P}^2 + \left(\mathsf{Z}_{13}\mathsf{T}^3 + \mathsf{Z}_{12}\mathsf{T}^2 \right. \\ &\quad + \mathsf{Z}_{11}\mathsf{T} + \mathsf{Z}_{10} \right) \mathsf{P} + \left(\mathsf{Z}_{03}\mathsf{T}^3 + \mathsf{Z}_{02}\mathsf{T}^2 + \mathsf{Z}_{01}\mathsf{T} + \mathsf{Z}_{00} \right) \right] \end{split}$$

Table 2 represents the values of the 36 constant coefficients of the above correlation.

5. Principles of sound speed calculation

As discussed above, in the proposed natural gas mass flow metering, the UFM measures sound speed in natural gas stream and the corresponding equation based on which a UFM measures sound speed was presented. However, as it was explained before, what has been provided by NIGC is only the information about compositions of different natural gas fields. Therefore, by employing the mixture compositions as well as different temperature and pressure ranges as the input information of AGA8 EOS, the authors produced a large database including the sound speed values in different temperatures and pressures for each of the gas mixtures. In this section, the thermodynamic principles based on which AGA8 EOS calculates sound speed are presented briefly. The general

Table 2	
The values of constant coefficients in Equation (11).	

.....

х	X X ₂				X ₁				X ₀			
	X ₂₃	X ₂₂	X ₂₁	X ₂₀	X ₁₃	X ₁₂	X ₁₁	X ₁₀	X ₀₃	X ₀₂	X ₀₁	X ₀₀
	8.429e-12	-1.829e-9	1.775e-7	-9.495e-6	-4.614e-11	1.157e-8	-1.368e-6	9.159e-5	-2.162e-11	6.403e-9	-1.711e-6	0.0006201
Y	Y ₂				Y ₁				Yo			
	Y ₂₃	Y ₂₂	Y ₂₁	Y ₂₀	Y ₁₃	Y ₁₂	Y ₁₁	Y ₁₀	Y ₀₃	Y ₀₂	Y ₀₁	Y ₀₀
	-6.576e-9	1.541e-6	-0.0001544	0.008268	2.488e-8	-6.724e-6	0.000859	-0.06548	1.045e-8	-2.461e-6	0.0007038	-0.5885
Z	Z2				Z1				Zo			
	Z ₂₃	Z ₂₂	Z ₂₁	Z ₂₀	Z ₁₃	Z ₁₂	Z ₁₁	Z ₁₀	Z ₀₃	Z ₀₂	Z ₀₁	Z ₀₀
	1.671e-6	-0.0003615	0.03341	-1.744	-3.987e-6	0.0009976	-0.1237	10.96	-5.633e-7	-2.04e-5	0.05414	154.6

format of sound speed calculation formula is:

$$\mathsf{C} = \sqrt{\left(\frac{\partial \mathsf{P}}{\partial \rho}\right)_{s}} \tag{12}$$

In which, s refers to entropy. Using this equation and taking mathematical relationship of partial differentials into account, one could re-write the above equation as:

$$C^{2} = \frac{1}{MW} \frac{\left(\frac{\partial P}{\partial T}\right)_{s}}{\left(\frac{\partial \rho_{m}}{\partial T}\right)_{s}}$$
(13)

Also, from Maxwell's relations and differential forms of combined first and second laws of thermodynamics, one has (Bejan, 2006):

$$\left(\frac{\partial P}{\partial T}\right)_{s} = \frac{C_{Pm}}{T\left(\frac{\partial v_{m}}{\partial T}\right)_{P}}$$
(14)

And,

$$\left(\frac{\partial \rho_{m}}{\partial T}\right)_{s} = C_{vm} \frac{\rho_{m}^{2}}{T\left(\frac{\partial P}{\partial T}\right)_{vm}}$$
(15)

Where, v_m is molar specific volume. Also, C_{vm} and C_{pm} are respectively molar heat capacity at constant pressure and constant volume and could be calculated by:

$$C_{\rm vm} = \left(\frac{\partial u_{\rm m}}{\partial s_{\rm m}}\right)_{\rm v_{\rm m}} \left(\frac{\partial s_{\rm m}}{\partial T}\right)_{\rm v_{\rm m}} \tag{16}$$

$$C_{pm} = C_{vm} + T \left(\frac{\partial v_m}{\partial T}\right)_p \left(\frac{\partial P}{\partial T}\right)_{v_m}$$
(17)

Finally, taking the above formulation into account, one has:

$$C^{2} = \frac{1}{MW} \times \frac{C_{pm}}{C_{vm}\rho_{m}^{2}} \frac{\left(\frac{\partial P}{\partial T}\right)_{\rho m}}{\left(\frac{\partial v_{m}}{\partial T}\right)_{P}}$$
(18)

6. Validation of the presented novel correlation

Two basic metrics, the MAE and MAPE, presented in the following equations, are used to compare and validate the performance of the presented correlation (Kusiak et al., 2009).

$$MAE = \frac{1}{N} \sum_{i=1}^{N} |\overline{y}_i - y_i||$$
(19)

$$MAPE = \frac{1}{N} \sum_{i=1}^{N} \left(\left| \frac{\overline{y}_i - y_i}{y_i} \right| \right) \times 100\%$$
(20)

Where, N is the number of test data points used to validate the performance of the correlation and \hat{y} and y are respectively the predicted and the observed value of a variable, i.e., the idiomatic and actual molecular weights. The small values of the MAE and MAPE imply superior performance of the corresponding correlation. It should be mentioned that the comparison is carried out between the idiomatic and the actual molecular weight of natural gas mixture in the pressure and temperature ranges which widely occur in Iran natural gas transmission pipelines; i.e. 0.1 MPa < P < 1.8 MPa, -20 °C < T < 80 °C.

7. Results and discussion

The results have been divided into two parts. In first part, the variation of idiomatic molecular weight against pressure, temperature and sound speed is presented. Fig. 4 shows the idiomatic molecular weight variations against sound speed and temperature for a constant pressure. In fact, this figure shows the values of idiomatic molecular weight calculated by Equation (11) for different temperatures and sound speeds which could be applied for every natural gas mixture. It should be noted that the correlation performance is illustrated for P = 1 MPa as a sample point in



Fig. 4. The idiomatic molecular weight variations versus sound speed changes for different temperatures in P=1~MPa.

order to avoid presenting several similar figures.

According to the figure, a regular decrease for the idiomatic molecular weight by increasing sound speed value is observed. Also, evidently, temperature growth affects idiomatic molecular weight value so that higher temperatures lead to higher idiomatic molecular weight values at constant pressures and sound speeds.

Comparing the idiomatic molecular weights at different temperatures, pressures and sound speeds with the actual values in the reference database reveals that the presented correlation is considerably reliable. To prove this reliability the following figures are presented. Figures 5–10 are presented in order to make a comparison between the actual molecular weights (calculated by AGA8 EOS based on its compositions) and the idiomatic molecular weight (calculated by Equation (11)) for three random selected gases (i.e. Qeshm, Aghar and Gonbadly), an intentionally selected field (i.e. Bidboland which is a sour gas and one could then evaluate the performance of the proposed equation for sour gases) as well as two sample gases (i.e. sample 1 which is pure methane and sample 2 which consists of 80% methane and 20% ethane). The black solid lines in the following figures refer to the actual molecular weight of the corresponding field.

Fig. 5 shows that the correlation estimates more accurate values in higher pressures and the accuracy is affected as pressure decreases while temperature variation doesn't affect the prediction accuracy considerably. Regarding the figure, the highest values of deviation for P = 0.1 MPa and P = 1.8 MPa are about 0.2 and 0.06, respectively.

Considering Fig. 6, similar to the results obtained for Qeshm, for Aghar also, idiomatic molecular weight value decreases as pressure increases while temperature change doesn't affect the idiomatic molecular weight value considerably. In the meantime, in contrast with Qeshm, lower prediction deviations could be expected for Aghar in lower pressures and calculation error increases from almost 0.1 in the lowest pressure up to almost 0.2 in the highest pressure level.

According to Fig. 7, which has been presented for Gonbadly, the correlation performance is extremely similar to its performance for Aghar. The lower pressure the natural gas stream has, the more accurate molecular weight values are obtained. The deviation doesn't exceed 0.09 in P = 0.1 MPa while the maximum deviation, which occurs in P = 1.8 MPa is almost 0.27. The average error value is below 0.15.

Fig. 8 shows the performance of the correlation in calculating



Fig. 5. Comparing the actual and idiomatic molecular weights for Qeshm.



Fig. 6. Comparing the actual and idiomatic molecular weights for Aghar



Fig. 7. Comparing the actual and idiomatic molecular weights for Gonbadly



Fig. 8. Comparing the actual and idiomatic molecular weights for Bidboland as a sour gas field.

the molecular weight of Bidboland as a sour natural gas. According to the figure, although the difference between the actual value and the predicted value of molecular weight is more comparing to the three previous fields, the accuracy is still acceptable as maximum deviation which is observed in the lowest temperature and middle range pressures doesn't exceed 0.29 and the average deviation is almost 0.2.

Fig. 9 also illustrates the performance of equation for molecular weight calculation for pure methane as a sample field. According to the figure, the predicted values of molecular weight for pure methane are extremely close to the actual values so that the prediction deviation doesn't exceed 0.1 in any case.

Fig. 10, however, shows that the prediction deviation could rise up to about 0.3 in high pressures for sample 2 and even the average error for this sample gas is almost 0.25 which is higher than all other considered fields. Note that natural gas mainly comprises methane and the behavior of a gas with only 80% methane in its compositions is definitely less similar to an actual natural gas. That's why the overall deviation in molecular weight prediction for sample 2 is bigger in comparison with the other considered compositions.

As a whole, it was observed that molecular weight prediction accuracy is much more affected by pressure variation than temperature change. Although, by far, the accuracy of the correlation is evidently proved as the maximum deviation in molecular weight prediction is below 0.3 which is really impressive, since the main goal of this work is to calculate natural gas mass flow rate by using AGA8 EOS, so the equation proficiency should also be assessed in density prediction directly. In the following figures, the actual and predicted density values are compared for five fields of natural gases considered in this study. In fact, as it was explained before, for calculating the actual density values, temperature, pressure and actual molecular weight values are given to the AGA8 EOS and it could calculate the exact value of density, on the other hand, for calculating the predicted value of density, in addition to pressure and temperature values, this time, the predicted values of molecular weight of each natural gas (calculated by Equation (11)) is given to the AGA8 EOS to generate a new density value.

Figures 11–15 present the actual and calculated densities of three other random selected natural gas fields (Sarkhoon, Pars and Khangiran) as well as the two chosen sample gases. Note that these figures have been presented to show density prediction accuracy



Fig. 9. Comparing the actual and idiomatic molecular weights for Sample $1-\mbox{Pure}$ Methane.



Fig. 10. Comparing the actual and idiomatic molecular weights for Sample 2.



Fig. 11. Actual/predicted density in different temperatures and pressures for Khangiran



Fig. 12. Actual/predicted density in different temperatures and pressures for Pars.



Fig. 13. Actual/predicted density in different temperatures and pressures for Sarkhoon



Fig. 14. Actual/predicted density in different temperatures and pressures for Pure Methane.



Fig. 15. Actual/predicted density in different temperatures and pressures for Sample 2.

variation by pressure increase in low $(-10 \degree C)$, medium $(40 \degree C)$, and high $(80 \degree C)$, temperatures. As all the figures prove, despite the slight observed deviations in predicting of molecular weight values, density calculation accuracy is even much more impressive (just under 0.5% in the worst cases). In other word, the prediction deviations in molecular weight prediction stage are so slight that their effects on density calculation are negligible.

Although, the super accuracy of the proposed metering method is easily observable from the above graphs and having a glance on the density comparison figures reveals this fact, however, presenting an error reporter graph as a common method for accuracy evaluation seems to be necessary yet. To this aim, the following figure (Fig. 16) exhibits the density prediction error by the proposed correlation relative to the actual densities of different natural gas fields including the two sample gases for three temperatures (low, medium and high) from the lowest possible pressure to the highest levels of pressure in metering unit of CGSs. As the figure shows, the error doesn't exceed 0.5% anywhere, while for more than 80% of the states the deviation is even below 0.3% and even the average error is lower than 0.25%. It is noteworthy here that the error observed in Ref. (Farzaneh-Gord et al., 2015a) came up to 1.2% in some points and the average error was in range of 0.45–0.50%.

As more professional methods of proficiency evaluation, two criterions were used to illustrate the deviation of the values predicted by the correlation from the practical values. Figs. 17 and 18 illustrate the results of MAE and MAPE analysis on the presented correlation performance, respectively. These figures also show the MAE and MAPE values in low, moderate and high temperatures for five different natural gas fields.

Expectedly, the results of this survey are in accordance with the density prediction figures and simple error reporter graph. Here also the best performance of correlation is associated with Khangiran while the worst calculation accuracy is for Sample 2. Note that even for Sample 2 as the worst case, which acts similar to a sour gas, both MAPE and MAE are still in very good ranges that prove the adequacy of the presented method.

8. Conclusion

In this work, a novel correlation for calculating natural gas molecular weight was developed by which natural gas mass flow meter passing through a CGS could be measured. The main advantage of the presented method is that the correlation is only a functional of natural gas temperature, pressure and sound speed and as a result, there is no need to any information about the



Fig. 16. Density prediction error density in different temperatures and pressures.



Fig. 17. MAE for the novel correlation in various temperature, pressure and sound speed ranges.





natural gas compositions. This correlation was developed based on data mining approaches on a database including four of main natural gas fields of Iran and its validity was investigated for 8 other natural gas fields. The molecular weight value calculated by this equation along with natural gas stream temperature and pressure are then given to AGA8 EOS to calculate the natural gas density. The proficiency of this equation was compared to the previous correlation developed for the same objective. Simple error assessment method shows that the maximum deviation in density prediction doesn't exceed 0.5% and average error is below 0.25% while by previous correlation the maximum error was well over 1.2% and the average deviation was almost 0.5%. Also, MAPE and MAE error analysis methods were used as two more criterions to better evaluate the performance of the correlation. Compatible with the results of simple error analysis, the overall MAPE and MAE values are also lower than the values given by the previous proposed correlation and in super satisfactory ranges (MAE is 0.04 for the worst case and the MAPE value associated with the poorest performance of the correlation is only 0.035). As a whole, taking the results of this study into account, one could easily notice that not only the performance of correlation presented in this work for calculating natural gas mass flow rate passing through a CGS is totally reliable, but also its accuracy almost doubles in comparison with the most recent correlation presented for the same objective.

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