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DEVELOPING NOVEL CORRELATIONS FOR CALCULATING NATURAL GAS THERMODYNAMIC PROPERTIES

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Natural gas is a mixture of 21 components and it is widely used in industries and homes. Knowledge of its thermodynamic properties is essential for designing appropriate processes and equipment. This paper presents simple but precise correlations of how to compute important thermodynamic properties of natural gas. As measuring natural gas composition is costly and may not be effective for real time process, the correlations are developed based on measurable real time properties. The real time properties are temperature, pressure and specific gravity of the natural gas. Calculations with these correlations are compared with measured values. The validations show that the average absolute percent deviation (*AAPD*) for compressibility factor calculations is 0.674%, for density is 2.55%, for Joule-Thomson coefficient is 4.16%. Furthermore, in this work, new correlations are presented for computing thermal properties of natural gas such as enthalpy, internal energy and entropy. Due to the lack of experimental data for these properties, the validation is done for pure methane. The validation shows that *AAPD* is 1.31%, 1.56% and 0.4% for enthalpy, internal energy and entropy respectively. The comparisons show that the correlations could predict natural gas properties with an error that is acceptable for most engineering applications.

Keywords: natural gas, thermodynamic properties, novel correlations, real time properties

1. INTRODUCTION

Natural gas is a naturally occurring and complex mixture of hydrocarbons with a minor amount of inorganic compounds. Due to rich natural gas resources as well as lower emissions of greenhouse gases than in other fossil fuels, natural gas has many applications in homes and industries. Natural gas is processed and transported before reaching its end users. Knowledge of thermodynamic properties of the natural gas is essential for designing appropriate processes and equipment.

The thermodynamic properties of natural gas could be obtained by laboratory techniques, employing Equations of State (EOS) or utilising correlations. Laboratory techniques have a high accuracy, but some thermodynamic properties of natural gas such as entropy, enthalpy and internal energy, are not measurable. The cost and difficulty of launching devices are other negative factors in reducing the use of laboratory techniques. By employing EOS or correlations, all thermodynamic properties of natural gas mixture could be calculated with acceptable accuracy and without spending much time. However, there are many places in gas industries in which real time natural gas properties are needed. As discussed, real time gas composition measurements are costly and may not be applicable, so it is necessary to develop correlation based on real time measurable property.

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In the past studies, many correlations for calculating thermodynamic properties of natural gas such as compressibility factor, density and viscosity, has been presented. In each of these correlations, each thermodynamic property is a functional of reduced properties such as reduced pressure, reduced volume, and reduced temperature.

For calculating compressibility factor of natural gas, the most widely accepted correlation has been presented by the Standing and Katz (S-K) (Standing and Katz, 1942) *z*-factor chart. The S-K chart was developed using data for binary mixtures of methane with propane, ethane, butane, and natural gases having a wide range of composition. None of the gas mixtures molecular weights exceed 40.

In recent years, most studies for calculating compressibility factor of natural gas have been done by employing correlations. Elsharkawy et al. (2001) presented a new model for calculating gas compressibility factor based on compositional analysis of 1200 compositions of gas condensates. Also Elsharkawy (2004) presented efficient methods for calculating compressibility factor, density and viscosity of natural gases. This model is derived from 2400 measurements of compressibility and density of various gases. Papp Correlation (Najim, 1995), Shell Oil Company Correlation (Kumar, 2004) and Beggs and Brill Correlation (Beggs and Brill, 1973) are direct relations and Hall-Yarborough Correlation (Yarborough and Hall, 1974), Dranchuk and Abou-Kassem Correlation (Dranchuk and Abou-Kassem, 1975) are iterative relations for calculating compressibility factor of natural gas. New correlation for compressibility factor of natural gas has been presented by Heidaryan et al. (2010) and Azizi et al. (2010). Heidaryan et al. (2010) correlation has 1.660 of average absolute percent deviation (*AAPD*) versus Standing and Katz (1942) chart.

There are many other correlations to calculate the density of natural gas. Some of the most important studies include: Dranchuk and Abou-Kassem (1975) developed a gas density correlation using 1500 data points, including pure gases and gas mixtures from different sources. They developed their EOS based on a Han-Starling form of the Benedict-Webb-Rubin EOS, reporting an *AAPD* 0.486% when specifically used within the pseudo reduced pressure and temperature ranges of 0.2 to 30 and 1.0 to 3.0, respectively. Londono et al. (2002) presented simplified correlations for hydrocarbon gas density such as natural gas. Their calculations show *AAPD* 0.426% for 5960 data points and 0.821% for 8256 data points. AlQuraishia and Shokirb (2009) use Alternating Conditional Expectations (ACE) algorithm and presented a new density correlations for hydrocarbon gases and pure and impure gas mixtures.

Many studies have been done to calculate the viscosity of natural gas by presenting correlations. These include: Elsharkawy (2004) correlation, Guo et al. (1997) correlation, Londono et al. (2002) and Heidaryan et al. (2010). Bahadori and Vuthaluru (2009) have presented a novel correlation for estimation of hydrate forming condition of natural gas. Their calculations show *AAPD* of 0.2% compared to experimental data.

In this paper, we are developing novel correlations for calculating most thermodynamic properties of natural gas such as: compressibility factor (Z factor), density, Joule-Thomson coefficient and thermal properties such as: internal energy, enthalpy and entropy. Each thermodynamic property is a functional of pressure, temperature and specific gravity (molecular weight) of natural gas.

It should be noted that the correlations were developed by curve fitting to the values obtained from numerical methods based on AGA8 EOS (1992) standards. These methods were developed by the authors and were previously presented in Farzaneh-Gord et al. (2010), also in Marić (2005), Marić et al. (2005) and Marić et al. (2007).

2. THE NOVEL CORRELATIONS

In this section, the correlations have been developed based on temperature, pressure and specific gravity of natural gas. These 3 properties (temperature, pressure and specific gravity) are real time measurable properties. The specific gravity represents gas compositions in these correlations. Natural gas specific gravity is defined as:

$$\gamma = \frac{Mw}{28.966} \tag{1}$$

In Equation (1), γ is natural gas specific gravity, Mw is molecular weight of natural gas and 28.966 is molecular weight of air. The range of pressure and temperature which the correlations have been developed for, are as follows:

$$0.2 < P\,(\text{MPa}) < 25;\;\; 250 < T\,(\text{K}) < 350 \tag{2}$$

The range of the properties has been selected based on the most engineering applications in natural gas industries (such as compressed natural gas stations, compressor stations, etc).

The coefficients for the correlation have been developed based on the numerical values of each property obtained from the method presented in Farzaneh-Gord and Rahbari (2012). Farzaneh-Gord and Rahbari (2012) developed a detailed numerical procedure for thermodynamic property calculation of natural gas mixture using AGA8 equation of state. Each thermodynamic property has been considered as a function of three properties (pressure, temperature and natural gas specific gravity). Here, based on comprehensive efforts, the property values have been calculated for the range of pressure and temperature mentioned in Equation 2. The property values then calculated for various natural gas compositions by employing the method presented in (Farzaneh-Gord and Rahbari, 2012). Then a general function has been fitted to the values.

The developed correlations are presented in the common form of Equation (3). All the properties (except entropy and Joule-Thomson coefficient) could be calculated using Equation 3.

$$Properties\,(T',P',\gamma') = A_1(T',\gamma')P'^4 + A_2(T',\gamma')P'^3 + A_3(T',\gamma')P'^2 + A_4(T',\gamma')P' + A_5(T',\gamma') \tag{3}$$

Where $A_i(T',\gamma');i=1,...,5$ are defined as:

$$A(T',\gamma') = B_1(T')\gamma'^2 + B_2(T')\gamma' + B_3(T') \tag{4}$$

And $B_j(T');j=1,2,3$ for each $A_i(T',\gamma')$ are defined in Equation (5):

$$B(T') = C_1T'^2 + C_2T' + C_3 \tag{5}$$

T',P',γ' are functions of temperature, pressure and gas specific gravity respectively and defined as follows:

$$T' = \frac{T-300}{50},\; P' = \frac{P-13}{7.3598},\; \gamma' = \frac{\gamma-0.62541}{0.07894} \tag{6}$$

The entropy and Joule-Thomson coefficient are correlated with the following equation:

$$Properties(T',P',\gamma') = A_1(T',\gamma')P'^6 + A_2(T',\gamma')P'^5 + A_3(T',\gamma')P'^4 + A_4(T',\gamma')P'^3 + A_5(T',\gamma')P'^2 + A_6(T',\gamma')P' + A_7(T',\gamma') \tag{7}$$

In which, $A_i(T',\gamma');i=1,...,7$ are defined by Equation (4). The coefficients of Equations (3, 4, 5 or 7), for each thermodynamic property are given later on in this study.

To validate the correlation results, the correlation and available experimental values have been compared. The percent error and average absolute percent deviation (*AAPD*) have been employed as comparisons tools:

$$Error(\%) = \frac{Property_{Cor} - Property_{Exp}}{Property_{Exp}} * 100 \tag{8}$$

$$AAPD(\%) = \frac{1}{n}\sum \left| \frac{Property_{Cor} - Property_{Exp}}{Property_{Exp}} * 100 \right| \tag{9}$$

In Equations (8), (9); $Property_{Cor}$ is the correlation value for property which was calculated using the developed correlations, $Property_{Exp}$ is an available experimental value for the property and n is the number of data.

3. RESULTS AND DISCUSSION

3.1. Z factor and density

Table 1 shows coefficients of Equations (3), (4) and (5) for compressibility factor correlation (Z correlations). Figure 1 shows a comparison for compressibility factor values, calculated from the correlation and experimental data. According to Figure 1, the highest coefficient of determination R^2 is 0.9936. It can be realised there is a very good agreement between the correlation and experimental values.

Table 1. Coefficients of Equations (3), (4) and (5) for Z correlation

For A_1	C_1	C_2	C_3	For A_2	C_1	C_2	C_3
B_1	7.83E-05	-0.0004	0.000472	B_1	0.001295	-1.82E-03	0.000684
B_2	-0.00154	0.002711	-0.00142	B_2	-0.00435	0.004197	0.000466
B_3	-0.00761	0.010891	-0.00428	B_3	-0.00677	0.005037	0.002744
For A_3	C_1	C_2	C_3	For A_4	C_1	C_2	C_3
B_1	-0.00054	0.003027	-0.00496	B_1	-0.00376	0.006003	-0.00391
B_2	0.00705	-0.01451	0.011258	B_2	0.011882	-0.00957	-0.01053
B_3	0.039503	-0.07042	0.056829	B_3	0.016224	0.014308	-0.05559
For A_5	C_1	C_2	C_3				
B_1	-0.00017	-0.00271	0.006393				
B_2	-0.00515	0.020102	-0.03541				
B_3	-0.0524	0.15468	0.79878				

Table 2 shows mole percent of natural gases used in compressibility factor calculation and Table 3 shows the range of temperature and pressure and *AAPD* (%) for compressibility factor calculation. Figure 2 shows error percent for compressibility factor calculation according to Equation 8. According to Figure 2 the error percent generally is in the range of -3% to +3%. Also with an increasing molecular weight the error percent increases too. According to Table 3, *AAPD* for 259 data is found to be 0.674%. This value shows that the developed correlation for compressibility factor (*Z* factor) has a good accuracy in comparison with the experimental data.

Table 2. Mole percent of natural gas components used in Z calculation

NG8	NG7	Mix2	Mix1	Component
90.644	96.580	62.65	98.61	CH_4
3.134	0.269	12.09	1.09	N_2
0.466	0.589	-	0.3	CO_2
4.553	1.815	25.26	-	C_2H_6
0.833	0.405	-	-	C_3H_8
0.1	0.099	-	-	i-C_4H_{10}
0.156	0.102	-	-	n-C_4H_{10}
0.03	0.047	-	-	i-C_5H_{12}
0.045	0.032	-	-	n-C_5H_{12}
0.04	0.063	-	-	n-C_6H_{14}
17.6057	16.7810	21.0334	16.2574	Mw

Table 3. *AAPD* for Z calculations

Mixture	Reference	Number of Data	T Range [K]	P Range [MPa]	*AAPD* [%]
Mix1	McElroy et al. (1989)	44	303-333	1-12	0.187073
Mix2	Staby and Mollerup (1991)	93	275-345	0.2-25	0.941
NG7	Hwang et al. (1997)	61	250-325	0.2-10.5	0.596104
NG8	Hwang et al. (1997)	61	275-325	0.2-10.5	0.697901
Overall		259			0.674

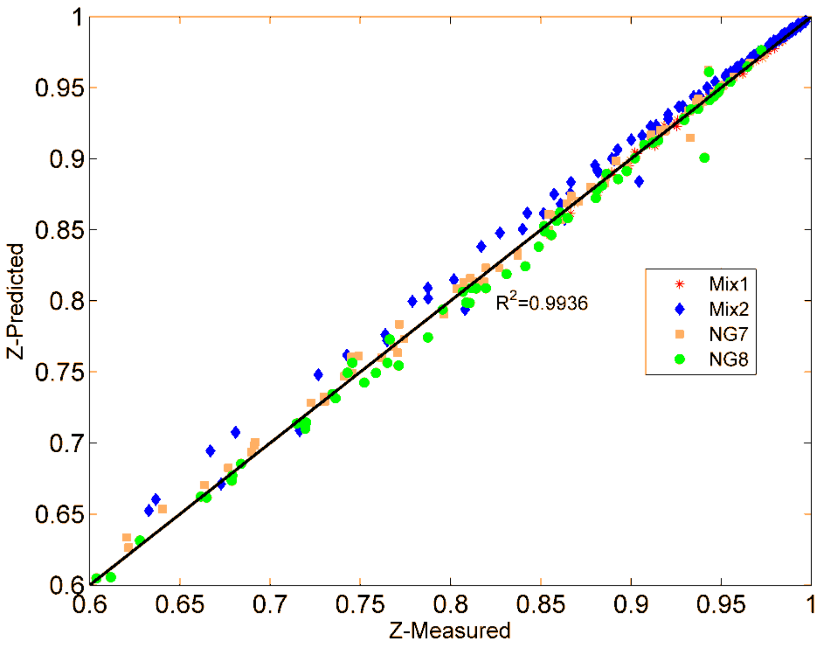

Fig. 1. Z predicted (correlations) versus Z measured (experimental)

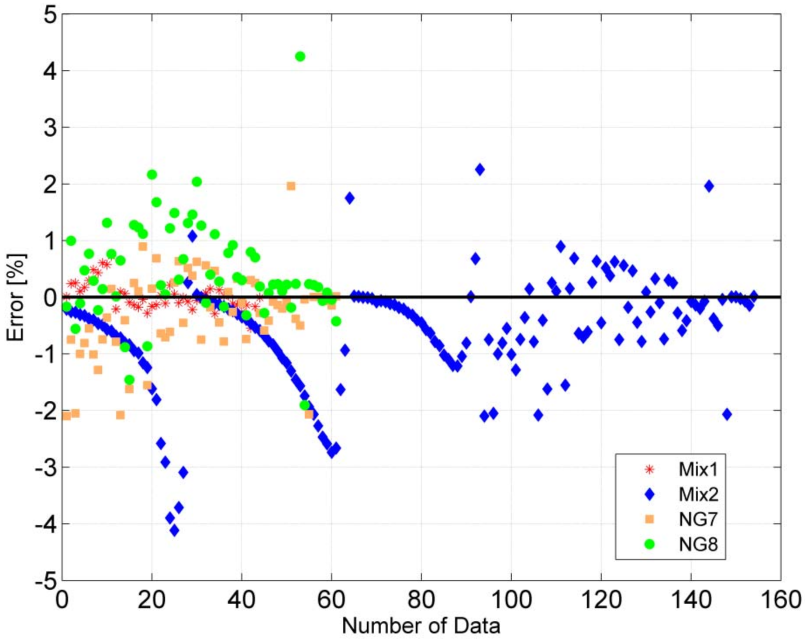

Fig. 2. Error percent in Z factor calculations

Table 4 shows coefficients of Equations (3), (4) and (5) for density correlation. Figure 3 shows a comparison for density values, calculated from the correlation and experimental data. According to Figure 3, the highest coefficient of determination R^2 is 0.9952. It can be realised there is a very good agreement between the correlation and experimental values for density calculations.

Table 4. Coefficient of Equations (3), (4) and (5) for density correlation

For A_1	C_1	C_2	C_3	For A_2	C_1	C_2	C_3
B_1	-0.05526	0.15435	-0.13256	B_1	-0.18862	0.15832	0.119
B_2	1.7407	-1.9248	0.18575	B_2	0.072855	0.82626	-1.3017
B_3	3.1504	-3.4759	0.37415	B_3	-1.7437	4.1125	-3.6585
For A_3	C_1	C_2	C_3	For A_4	C_1	C_2	C_3
B_1	0.25149	-0.8673	1.0182	B_1	0.67253	-0.58572	-1.7529
B_2	-7.1057	8.3016	-1.2637	B_2	0.3058	-5.7102	14.733
B_3	-14.053	16.529	-3.6958	B_3	8.2435	-29.149	75.528
For A_5	C_1	C_2	C_3				
B_1	0.05925	0.95545	-4.4321				
B_2	7.67	-14.843	21.723				
B_3	22.282	-51.938	122.61				

Table 5 shows mole percent of natural gases used in density calculation and Table 6 shows the range of temperature and pressure and *AAPD* (%) for density calculation. Figure 4 shows the error percent for density calculation according to Equation 8. According to Figure 4, the error percent is generally between -4 and +4%. Also with an increasing molecular weight the error percent increases too. Error percent is lower for natural gases with lower molecular weight and in the temperature and pressure conditions close to the ideal gas. According to Table 6, *AAPD* for 167 data is found to be 2.55%. This value shows the developed correlation for density has acceptable accuracy in comparison with the experimental data.

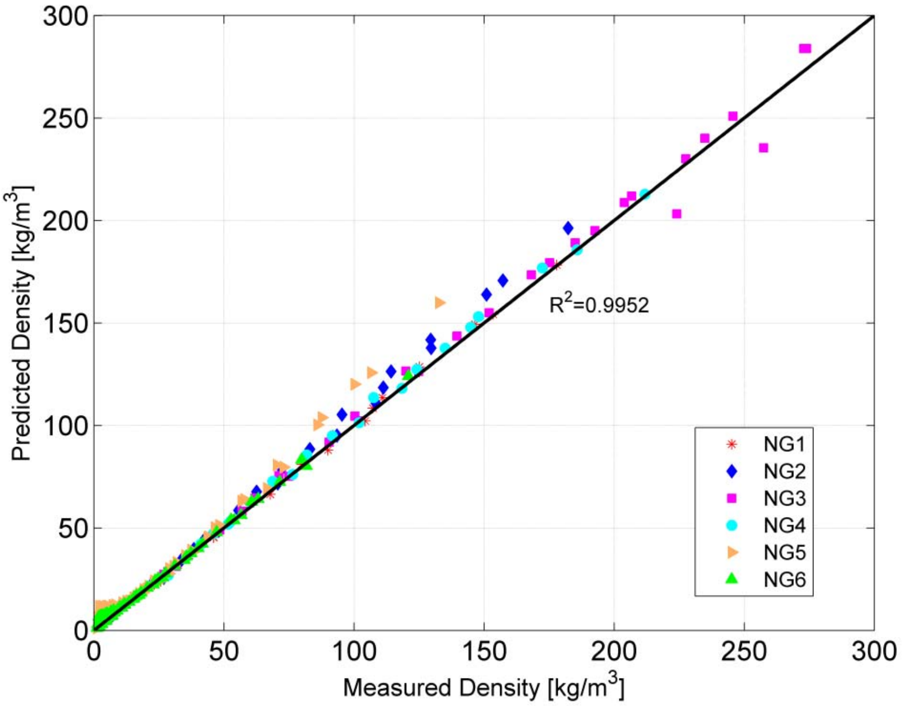

Fig. 3. Predicted density versus measured density (experimental)

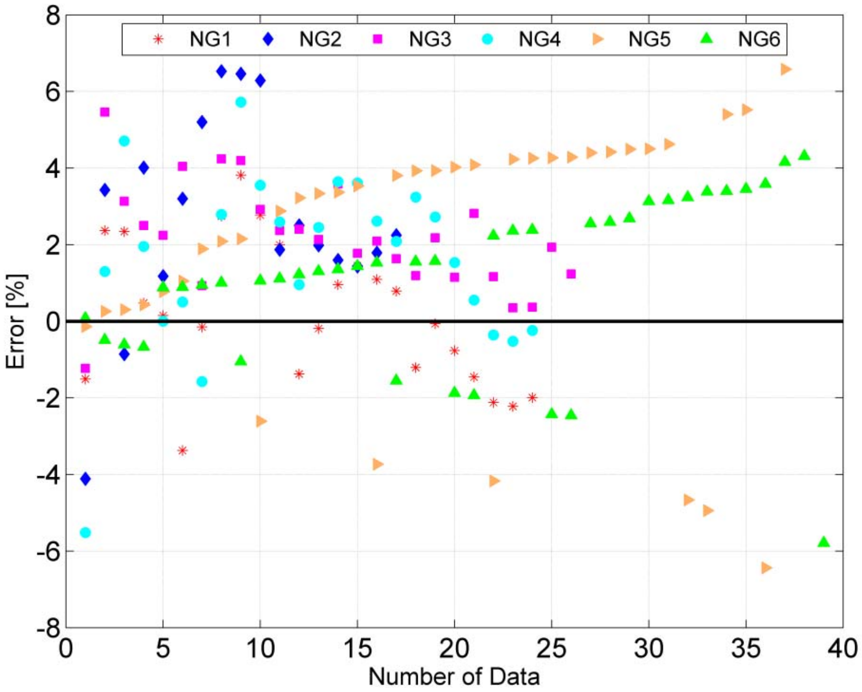

Fig. 4. Error percent in density calculations

Table 5. Mole percent of natural gas components used in density calculation

NG6	NG5	NG4	NG3	NG2	NG1	Component
85.898	81.299	90.362	90.991	92.436	98.352	CH_4
1.007	13.575	1.474	2.031	5.751	0.841	N_2
1.498	0.994	0.676	0.403	0.052	0.066	CO_2
8.499	3.294	5.708	2.949	1.285	0.511	C_2H_6
2.296	0.637	1.124	1.513	0.345	0.153	C_3H_8
-	-	0.011	-	-	-	O_2
-	-	0.015	-	-	-	He
0.351	0.101	0.301	0.755	0.041	0.021	i-C_4H_{10}
0.347	0.1	0.169	0.755	0.046	0.031	n-C_4H_{10}
0.051	-	0.059	0.299	0.015	0.008	i-C_5H_{12}
0.053	-	0.029	0.304	0.014	0.011	n-C_5H_{12}
-	-	0.058	-	0.012	0.005	n-C_6H_{14}
-	-	0.035	-	-	0.001	n-C_7H_{16}
-	-	0.008	-	-	0.0003	n-C_8H_{18}
18.7708	18.6713	17.8415	18.21067	17.08514	16.31391	Mw

Table 6. *AAPD* for density calculations

Mixture	Reference	Number of Data	*T* Range [K]	*P* Range [MPa]	*AAPD* [%]
NG1	Čapla et al. (2002)	24	253.15-323.15	1-15	1.58
NG2	Čapla et al. (2002)	17	253.15-323.15	1-15	3.22
NG3	Patil et al. (2007)	26	270-340	2-25	2.28
NG4	Čapla et al. (2002)	24	253.15-323.15	1-15	2.28
NG5	Hwang et al. (1997)	37	250-325	0.2-10.5	3.48
NG6	Hwang et al. (1997)	39	275-325	0.2-10.5	2.1
Overall		167			2.55

3.2. Joule-Thomson coefficient

Joule-Thomson (JT) coefficient is one of the most important properties of natural gas in industry process analysis. The role of this factor is very important in the process of throttling valves. Joule-Thomson coefficient is defined as follows:

$$\mu_{JT} = \left(\frac{\partial T}{\partial P}\right)_h \tag{10}$$

Where, μ_{JT} is Joule-Thomson coefficient, *P* is pressure, *h* is enthalpy and *T* is temperature. So far there has been no correlation for calculating Joule-Thomson (JT) coefficient. Table 7 shows coefficients of Equations (7), (4) and (5) for Joule-Thomson coefficient correlation. To improve the accuracy of the calculations, Equation 7 has been used instead of Equation 3. Figure 5 shows a comparison for Joule-Thomson (JT) coefficient calculated from the correlation and experimental data. According to Figure 5, the highest coefficient of determination R^2 is 0.9829. This value shows that the developed correlation for Joule-Thomson (JT) coefficient has acceptable accuracy compared with the experimental data.

Table 7. Coefficients of Equations (7), (4) and (5) for Joule-Thomson coefficient correlation

For A_1	C_1	C_2	C_3	For A_2	C_1	C_2	C_3
B_1	-0.00894	0.010027	-0.00124	B_1	-0.00276	0.001671	0.001501
B_2	0.037372	-0.04141	0.004233	B_2	3.85E-02	-0.02912	-0.01046
B_3	0.08171	-0.08658	0.005195	B_3	1.01E-05	0.021619	-0.02514
For A_3	C_1	C_2	C_3	For A_4	C_1	C_2	C_3
B_1	0.049832	-0.05904	0.011103	B_1	0.011734	-0.00139	-0.01664
B_2	-0.22478	0.25142	-0.02822	B_2	-0.12584	0.063054	0.077993
B_3	-0.47449	0.50904	-0.03746	B_3	0.10902	-0.28586	0.23611
For A_5	C_1	C_2	C_3	For A_6	C_1	C_2	C_3
B_1	-0.09496	0.12545	-0.03947	B_1	-0.0067	-0.03627	0.089453
B_2	0.42316	-0.48883	0.066863	B_2	0.05813	0.12006	-0.30289
B_3	0.90366	-0.97836	0.058173	B_3	-0.47252	1.2687	-1.6419
For A_7	C_1	C_2	C_3				
B_1	0.042	-0.0597	0.0358				
B_2	-0.1959	0.2151	0.1854				
B_3	-0.4659	-0.148	2.8769				

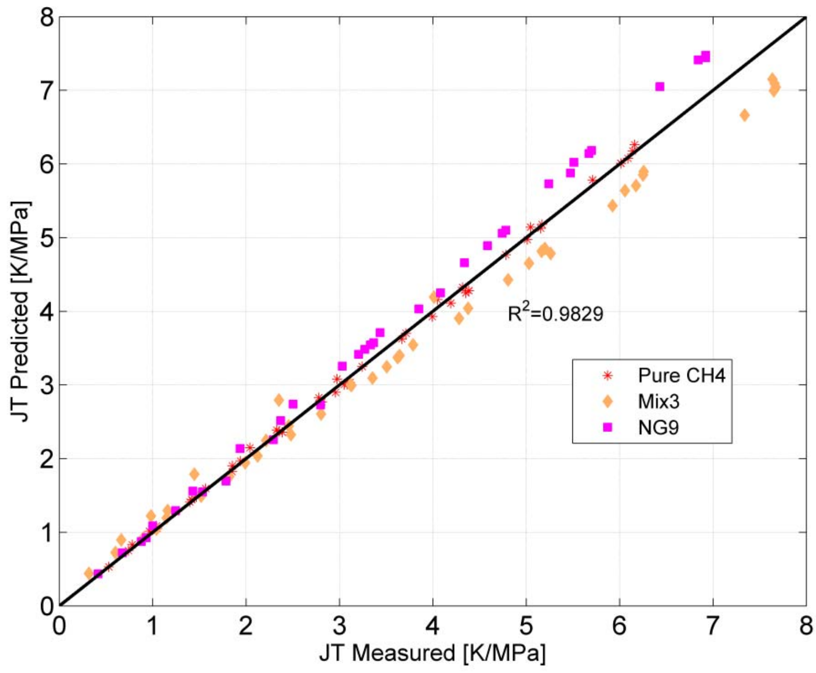

Fig. 5. JT predicted (correlation) versus JT measured (experimental)

Table 8 shows mole percent of natural gases used in Joule-Thomson (JT) coefficient calculation and Table 9 shows the range of temperature and pressure and *AAPD* (%) for JT coefficient calculation. Figure 6 shows the error percent for JT coefficient calculation according to Equation 8. According to Figure 6, the error percent generally between -8 and +8%. Also with an increasing molecular weight the error percent increases too. Error percent is lower for natural gases with lower molecular weight and in the temperature and pressure conditions close to the ideal gas. According to Table 9, *AAPD* for 112 data is found to be 4.16%. So one could conclude that the proposed correlation has acceptable accuracy for calculating JT coefficient.

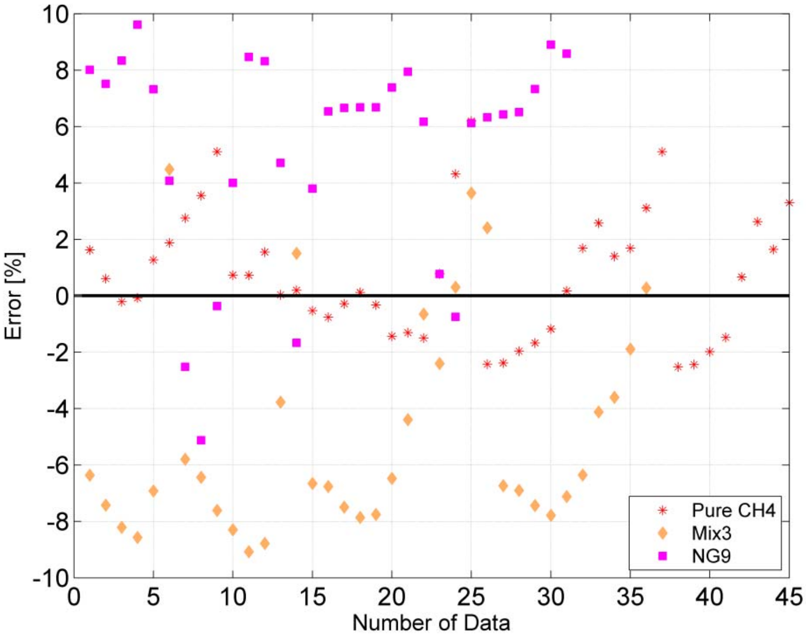

Fig. 6. Error percent in Joule-Thomson (JT) coefficient calculations

Table 8. Mole percent of natural gas components used in heat capacity at constant pressure calculations

NG9	Mix3	Pure CH4	Component
79.942	85	100	CH_4
9.939	-	-	N_2
2.09	-	-	CO_2
5.029	15	-	C_2H_6
3	-	-	C_3H_8
19.3643	18.14705	16.043	Mw

Table 9. *AAPD* for Joule-Thomson calculations

Mixture	Reference	Number of Data	*T* Range [K]	*P* Range [MPa]	*AAPD* [%]
Pure CH4	Ernst et al. (2001)	45	250-350	0.6-25	1.78
Mix3	Ernst et al. (2001)	36	250-350	0.6-25	5.6201
NG9	Ernst et al. (2001)	31	250-350	0.6-25	5.9256
Overall		112			4.1601

3.3. Enthalpy

Enthalpy is one of the thermal properties of natural gas. The role of this property is very important in employing the first law of thermodynamics for open systems. To the authors' knowledge, there is no proposed correlation for calculating enthalpy. Table 10 shows coefficients of Equations (3), (4) and (5) for enthalpy correlation. Figure 7 shows a comparison for enthalpy, calculated from the correlation and the experimental data. According to Figure 7, the highest coefficient of determination R^2 is 0.9999. This value shows the developed correlation for enthalpy has good accuracy in comparison with the experimental data. Due to the lack of experimental data, the validation is done for pure methane.

Table 10. Coefficients of Equations (3), (4) and (5) for enthalpy correlation

For A_1	C_1	C_2	C_3	For A_2	C_1	C_2	C_3
B_1	0.23536	-0.38033	0.19855	B_1	0.43936	-0.45315	-0.02597
B_2	-0.78975	1.0733	-0.32314	B_2	-1.178	0.91628	0.39662
B_3	-3.0909	3.8865	-1.0332	B_3	-0.4224	-1.2654	2.6406
For A_3	C_1	C_2	C_3	For A_4	C_1	C_2	C_3
B_1	-1.0239	2.0382	-1.8366	B_1	-1.1998	1.0624	1.6883
B_2	3.2382	-4.843	1.9398	B_2	3.5961	-2.8299	-1.5916
B_3	14.76	-21.626	12.979	B_3	-1.478	21.888	-67.311
For A_5	C_1	C_2	C_3				
B_1	0.502	-5.578	6.565				
B_2	-1.901	-6.156	-4.34				
B_3	-19.34	167.9	-131.2				

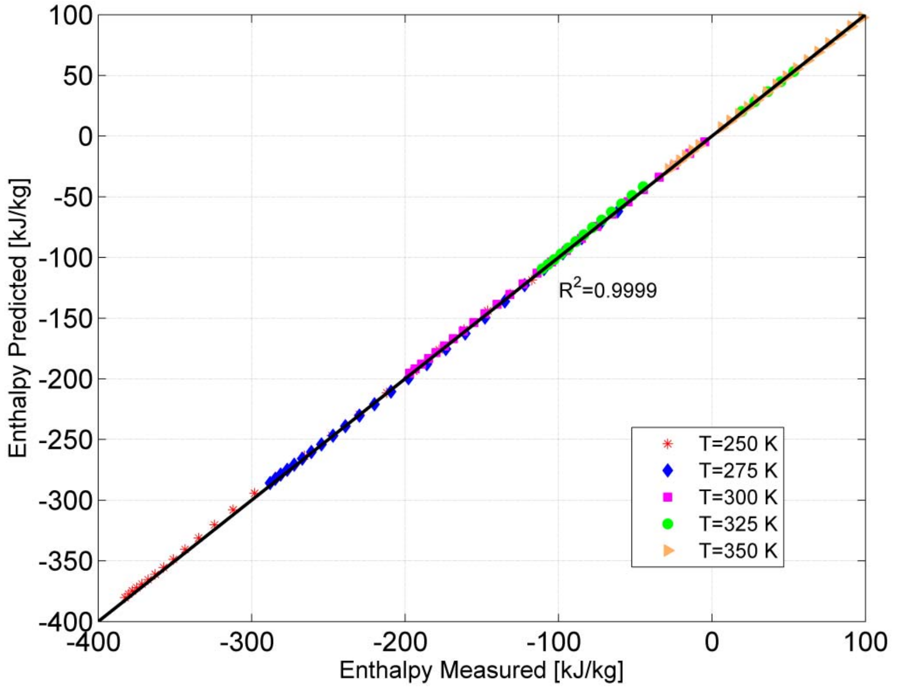

Fig. 7. Enthalpy predicted (correlation) versus enthalpy measured (experimental)

Table 11 shows the range of temperature and pressure and *AAPD* (%) for enthalpy calculation. Figure 8 shows error percent for enthalpy calculation. According to Figure 8, the error percent is generally between -2 and +8%. Furthermore, with an increasing temperature the error percent increases too. According to Table 11, *AAPD* for 116 data is found to be 1.31%. So, one can conclude that the correlation has very high accuracy for predicting the enthalpy of natural gas.

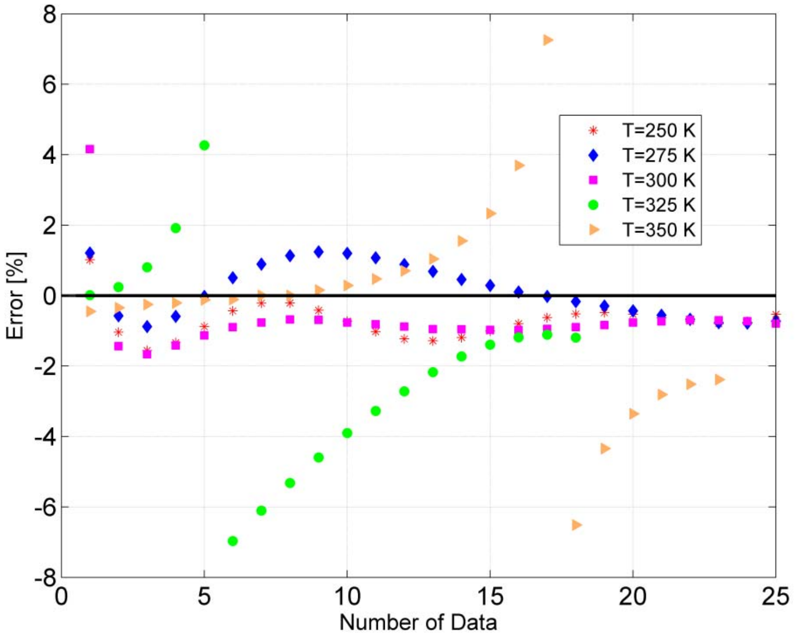

Fig. 8. Error percent in enthalpy calculations

Table 11. *AAPD* for enthalpy calculation for pure methane

	Ref	Number of Data	*T* Range [K]	*P* Range [MPa]	*AAPD* [%]
Pure CH_4 *Mw* = 16.043	Setzmann and Wagner (1991)	116	250-350	1-25	1.31

3.4. Internal Energy

Internal energy (u) is another thermal property of natural gas. The role of this property is very important in employing the first law of thermodynamics for close systems. There has not been any correlation for calculating internal energy of natural gas. Table 12 shows coefficients of Equations (3), (4) and (5) for internal energy correlation. Figure 9 shows a comparison between the correlated and measured values. According to Figure 9, the highest coefficient of determination R^2 is 0.9999. This shows the proposed correlation has high accuracy for predicting internal energy. Due to the lack of experimental data, the validation is done for pure methane.

Table 13 shows the range of temperature and pressure and *AAPD* (%) for internal energy calculation. Figure 10 shows error percent for internal energy calculation. According to Figure 10, the error percent is generally between -4 and +4%. Furthermore, with an increasing temperature the error percent increases too. According to Table 13, *AAPD* for 120 data is found to be 1.56%. This again shows the accuracy of the proposed correlation.

Table 12. Coefficients of Equations (3), (4) and (5) for internal energy correlation

For A_1	C_1	C_2	C_3	For A_2	C_1	C_2	C_3
B_1	0.25132	-0.3521	0.13108	B_1	0.25301	-0.18932	-0.13035
B_2	-0.80744	0.99402	-0.20444	B_2	-0.7492	0.44572	0.41918
B_3	-2.4667	2.8722	-0.49952	B_3	0.53947	-2.1242	2.4279
For A_3	C_1	C_2	C_3	For A_4	C_1	C_2	C_3
B_1	-1.0812	1.7895	-1.1521	B_1	-0.67335	0.18565	2.2516
B_2	3.292	-4.4129	1.324	B_2	2.4149	-1.2358	-1.2587
B_3	11.507	-14.898	5.592	B_3	-4.486	21.857	-60.922
For A_5	C_1	C_2	C_3				
B_1	0.6633	-5.804	5.535				
B_2	-2.234	-2.993	-2.703				
B_3	-15.888	129.5	-104.11				

Table 13. *AAPD* for internal energy calculation for pure methane

	Ref	Number of Data	*T* Range [K]	*P* Range [MPa]	*AAPD* [%]
Pure CH_4 *Mw* = 16.043	Setzmann and Wagner (1991)	120	250-350	1-25	1.56

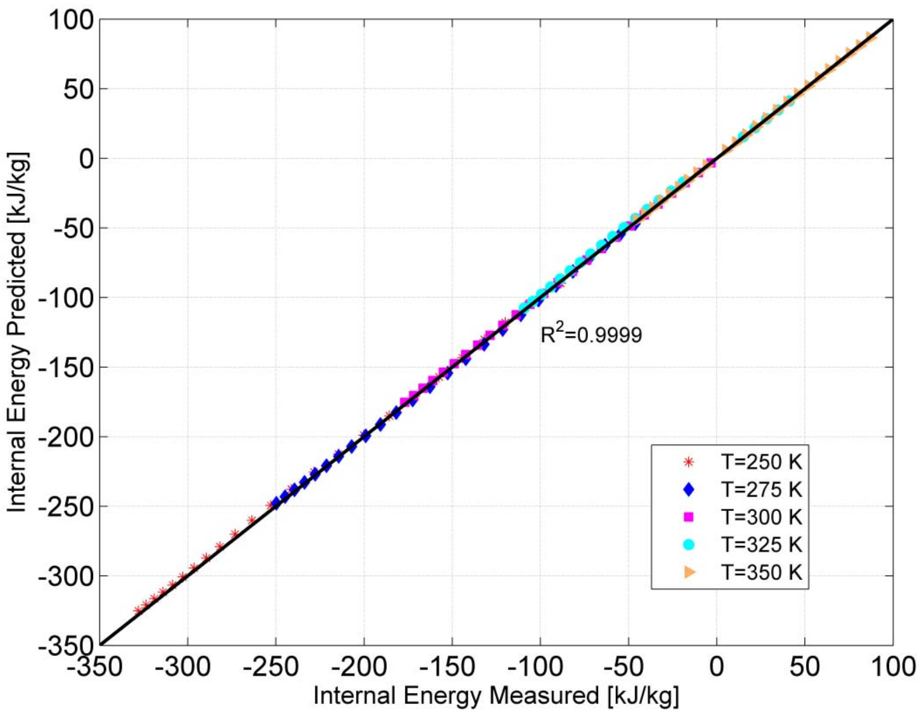

Fig. 9. Internal energy predicted (correlation) versus internal energy measured (experimental)

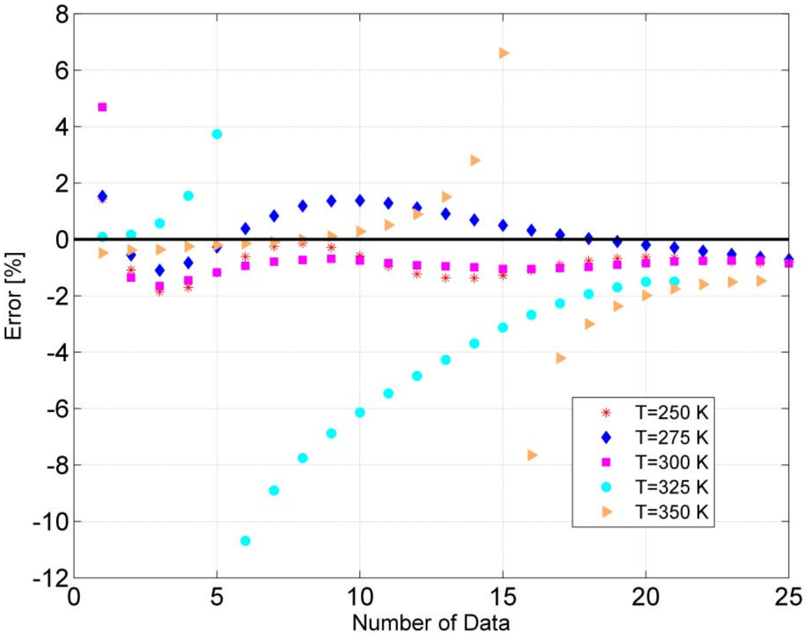

Fig. 10. Error percent in internal energy calculations

3.5. Entropy

Entropy (*s*) is another thermal property of natural gas. The role of this property is very important in the second law of thermodynamics and entropy generation for all processes. There is no previous correlation for calculating entropy. Table 14 shows coefficients of Equations (7), (4) and (5) for entropy correlation. To improve the accuracy of the correlation, Equation 7 has been used instead of Equation 3. Figure 11 shows a comparison between the experimental and the correlated values. According to Figure 11, the highest coefficient of determination, R^2, is 0.9999. This shows a very high accuracy in predicting entropy of natural gas using the developed correlation. Due to the lack of experimental data for this property, the validation is done for pure methane.

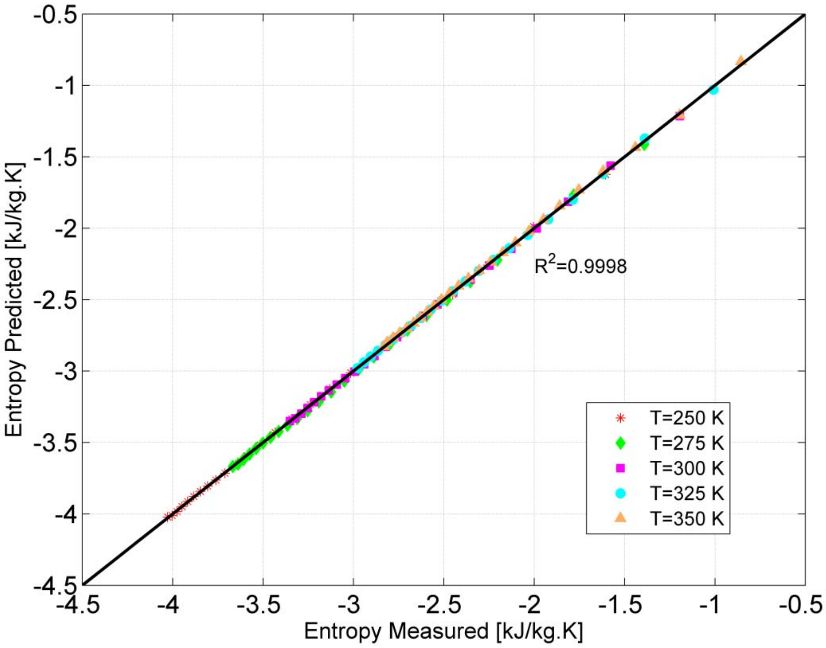

Fig. 11. Entropy predicted (correlation) versus entropy measured (experimental)

Table 14. Coefficients of Equations (7), (4) and (5) for entropy correlation

For A_1	C_1	C_2	C_3	For A_2	C_1	C_2	C_3
B_1	-0.00033	0.000423	0.000261	B_1	-0.00099	0.001026	-0.00057
B_2	0.000743	-0.001	-0.0026	B_2	0.003706	-0.00349	0.003969
B_3	0.004234	-0.00473	0.022844	B_3	0.003733	-0.00295	-0.03382
For A_3	C_1	C_2	C_3	For A_4	C_1	C_2	C_3
B_1	0.002197	-0.003	0.000394	B_1	0.004791	-0.00497	0.000461
B_2	-0.00586	0.007762	0.002631	B_2	-0.01618	0.014682	-0.00114
B_3	-0.0282	0.032628	-0.04156	B_3	-0.01318	0.005427	0.034677
For A_5	C_1	C_2	C_3	For A_6	C_1	C_2	C_3
B_1	-0.00528	0.00878	-0.0037	B_1	-0.00638	0.006062	-0.00097
B_2	0.015066	-0.02109	-0.00634	B_2	0.020652	-0.01787	0.032951
B_3	0.07261	-0.09597	0.13997	B_3	-0.0032	0.068045	-0.45239
For A_7	C_1	C_2	C_3				
B_1	0.00337	-0.0192	-0.17762				
B_2	-0.00491	-0.0196	0.47858				
B_3	-0.11575	0.57495	-2.2514				

Table 15 shows the range of temperature and pressure and *AAPD* (%) for entropy calculation. Figure 12 shows error percent for entropy calculation. According to Figure 12, the error percent is generally between -1 and +1%. According to Table 15, *AAPD* for 122 data is found to be 0.4%. This again shows a very high accuracy of the developed correlation for entropy prediction.

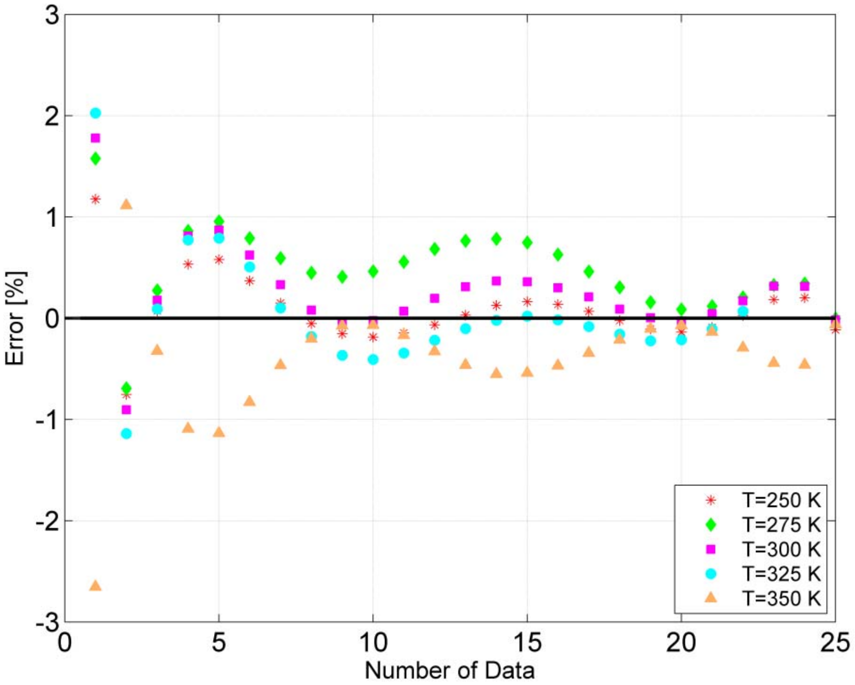

Fig. 12. Error percent in entropy calculations

Table 15. *AAPD* for entropy calculation for pure methane

	Ref	Number of Data	*T* Range [K]	*P* Range [MPa]	*AAPD* [%]
Pure CH_4 $Mw = 16.043$	Setzmann and Wagner (1991)	122	250-350	1-25	0.4

4. CONCLUSIONS

Given the current surge in natural gas businesses, trustworthy estimates of thermodynamic properties are necessary to design engineering processes. Accurate prediction of thermodynamic properties for natural gas is an essential requirement in optimum design and operation of most process equipment involved in petrochemical production, transportation, and processing. This work presents simple but precise correlations to compute important thermodynamic properties of natural gas. The correlations are developed based on measurable real time properties. The real time properties are temperature, pressure and specific gravity of the natural gas. The comparison between the measured and correlation values shows that the overall *AAPD* value is acceptable in most engineering applications. This proves that the presented correlation may be employed as trusted equations to compute natural gas thermodynamic properties.

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SYMBOLS

AAPD	average absolute percent deviation, %
A, B, C	Coefficient of correlations for each property, -
h	enthalpy, kJ/kg
Mw	molecular weight, kg/kmol
n	number of experimental data
P	pressure, MPa
s	entropy, kJ/(kg·K)
T	temperature, K
u	internal energy, kJ/kg
x	mole fraction of component, -
Z	compressibility factor, -

Greek symbols

γ	gas gravity
μ_{JT}	Joule-Thomson coefficient, K/MPa

Abbreviations

EOS	equation of state

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