

A NEW CORRELATION FOR ACCURATE ESTIMATION OF NATURAL GASES WATER CONTENT

Mohammad M. Ghiasi¹, Alireza Bahadori^{2*}

¹*Petroleum University of Technology, Ahwaz Faculty of Petroleum, Post Box: 63431, Ahwaz, Iran;* ²*Southern Cross University, School of Environment, Science and Engineering, Post Box 157, Lismore, NSW 2480, Australia; Corresponding author: alireza.bahadori@scu.edu.au*

Received December 1, 2013, Accepted November 15, 2014

Abstract

Accurate estimation of natural gas water content is very important and crucial for proper handling of many natural gas production and processing operations. In this paper, a new mathematical expression is developed for accurate estimation of the water content of sweet natural gas in equilibrium with liquid water for temperatures from 298.15 to 413.15 K as well as pressures between 3 to 80 MPa. The average absolute deviation percent is 0.86% and it proves the excellent agreement of predicted values using new correlation in comparison with reported data in the literature. The precision of new correlation to predict the water content of natural gas could not be provided by any of the other investigated methods. The excellent performance of the proposed correlation along with its simplicity and uncomplicatedness enable accurate and fast estimation of natural gas water content for any natural gas industrial applications.

Key words: Natural gas; water content; prediction; empirical correlation.

1. Introduction

Coexistence of water and natural gas in the reservoir will contribute to produce gas stream saturated by water vapor together with liquid water. Amount of water condensates depends on the surface and reservoir differences in pressure and temperature. Before delivery of produced gas from well to the pipelines, some processes include liquid separation, sweetening, and dehydration must be performed. Detail description of the gas treatment can be found elsewhere [14,22,31].

Water content is one of the extremely important factors affecting the design of gas treatment facilities. The water content also affects the injection rate of inhibitor in hydrate inhibition system for production/transmission pipelines. In addition, the rate at which corrosion occurs, determining the pipeline's lifetime, is in direct proportion to the existing water in the gas resulting in oxidation [2].

Due to the mentioned facts, accurate prediction of natural gas water content lead to safe and economic design of natural gas equipment. Calculation of such properties as viscosity and density of the gas phase represent another aspect of water content importance [43].

Available methods for estimation of natural gas water content can be categorized in two main groups: thermodynamic approaches, and empirical correlations. By applying the Raoult's law to water, the simplest thermodynamic model known as ideal model is written as follows:

$$y_w = \frac{x_w P^{sat}}{P} \quad (1)$$

where y_w and x_w are mole fractions of water in vapor and liquid phase, respectively; P is absolute pressure of the system, and P^{sat} is water vapor pressure at system temperature.

Based on this model Bukacek [6] and Mohammadi *et al.* [29] proposed separate correlations to estimate the water content of sweet natural gases. Bukacek [6] correlation is applicable at temperatures higher than 288.15 K [8,30], and proposed correlation of Mohammadi *et al.* [29]

is developed in the temperature range of 273.15 K and 477.59 K and pressures up to 14.40 MPa.

More complicated thermodynamic models are based on fugacity uniformity of each component in all phases of the system. The methods of Erbar *et al.* [13], Li and Firoozabadi [24], Chapoy *et al.* [10], Zirrahi *et al.* [43], and Chapoy [11] are such models. The presented method by Chapoy (2004), however, is derived by employing some assumptions. Hence, this method is a semi-empirical approach for estimating the natural gas water content. By using the equation of Chapoy [11], the water mole fraction in the gas phase is estimated as follows:

$$y_w = \left(\frac{P^{sat}}{\phi_w P} \right) \exp \left(\frac{v_w^L (P - P^{sat})}{RT} \right) \quad (2)$$

where v_w^L is water molar volume, and ϕ_w is fugacity coefficient of water in the gas phase. v_w^L and P^{sat} are estimated by the relations reported by Daubert and Danner [12] and McCain [27],

respectively. Chapoy [11] proposed the following equation to estimate ϕ_w :

$$\phi_w = \exp(BP + CP^2) \quad (3)$$

where B and C are temperature dependent functions as below:

$$B = a + \frac{b}{T} \quad (4)$$

$$C = c + \frac{d}{T} \quad (5)$$

where a , b , c , d are coefficients.

In addition to the thermodynamic and empirical methods, some charts have been provided in the literature (McKetta and Wehe [28], Robinson *et al.* [37], Campbell [9]; Wichert and Wichert [40]) for estimation of natural gas water content. In many standards, McKetta and Wehe [28] chart is recommended for estimation of sweet natural gas water content. [29]. This chart has been regenerated in many publications [8] like Gas Processors and Suppliers Association (GPSA) Engineering Book [1]. Since graphical based calculations need in most cases an interpolation, they are usually time consuming and tedious.

In view of this fact many authors such as Kobayashi *et al.* [21], Ning *et al.* [32], and Bahadori *et al.* [4] tried to develop a correlation representing the curves plotted in the McKetta and Wehe [28] chart. Kobayashi *et al.* [21] correlation is quite intricate and is applicable for pressures up to 14 MPa. The complicated dependency of coefficients of Ning *et al.* [32], and Bahadori *et al.* [4] correlations on pressure and temperature respectively makes these correlations nearly tedious tools.

In this study, first, an easy to use correlation will be presented for accurate predicting the water content of sweet natural gases based on the reproduced McKetta and Wehe chart [1]. Next, the capability of the new and Ning *et al.* [32] correlations in representing the McKetta and Wehe chart [1] will be evaluated.

Finally, precision of the new correlation will be compared with some available methods by employing previously published experimental data of water content for various gaseous systems in equilibrium with pure water.

2. Predictive tool development

To develop a reliable correlation capable to predict the water content of sweet natural gases, a total number of 312 data points have been extracted from McKetta-Wehe chart reproduced by GPSA Engineering Data Book [1]. In an attempt to present an easy to use, yet accurate correlation, saturated water content of sweet, lean natural gases, is assumed to be function of only temperature and pressure of the system, and the effect of gas composition on water content is assumed to be negligible. Table 1 shows the pressure, temperature, and water content operating ranges of collected data.

With the objective of generating an empirical correlation, a curve fitting process may be performed. Curve fitting is defined as finding an approximate function that describes the data points as a whole with the smallest error. This function does not have to go through all

the data points (Yang *et al.* [42]). The commonly used approximants are polynomials, trigonometric functions, and exponential functions (Hoffman [15]).

Table 1 Operating ranges of extracted data from McKetta-Wehe chart [20] for pressure, temperature, and water content

Variable	Minimum	Maximum
P (MPa)	3	80
T (K)	298.15	413.15
W (g/Sm ³)	0.150237	85.0697

The Weierstrass approximation theorem [7,15] which states that any continuous function can be approximated on a finite interval as closely as one wishes by a suitable polynomial, makes polynomials as the most frequently used general purpose for treating with functions on bounded domains midst other available approximating functions. The Weierstrass's theorem is proved in many different ways [19]. The properties of polynomials are described in detail by Quarteroni *et al.* [35]. In the present work, a bivariate polynomial of the following form is employed to model the water content of sweet natural gas as function of temperature and pressure.

$$z = a_0 + a_1x + a_2y + a_3x^2 + a_4y^2 + a_5xy + a_6x^3 + a_7y^3 + a_8x^2y + a_9xy^2 \quad (6)$$

In the development of desired correlation, all dependent and independent variables are investigated in logarithmic form. This decision is a consequence of this fact that the logarithmic functions are smooth and non-oscillatory equations that contribute to precise predictions [3]. Before the advent of computers these functions provided a means of easily performing many tedious computations. Figures 1 and 2 clearly demonstrate the usefulness of applying the logarithmic functions to simplify the modeling. As it shown Figure 2 looks like a thin flat plate while Figure 1 has more complicated shape. After this consideration, the final form of the proposed equation is as follows:

$$\log(W) = (A_1 \log(P) + A_2 \log(P)^2 + A_3 \log(P)^3) + (B_1 \log(T) + B_2 \log(T)^2 + B_3 \log(T)^3) + (C_1 \log(P) \times \log(T) + C_2 \log(P)^2 \times \log(T) + C_3 \log(P) \times \log(T)^2) + D \quad (7)$$

where W is water content in g/Sm³, P is pressure in MPa, T is temperature in K, and A_i , B_i , C_i , and D are coefficients.

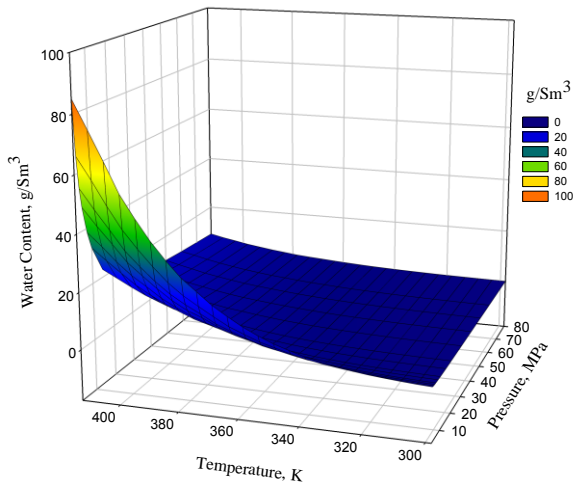


Figure 1 Water content as function of pressure and temperature

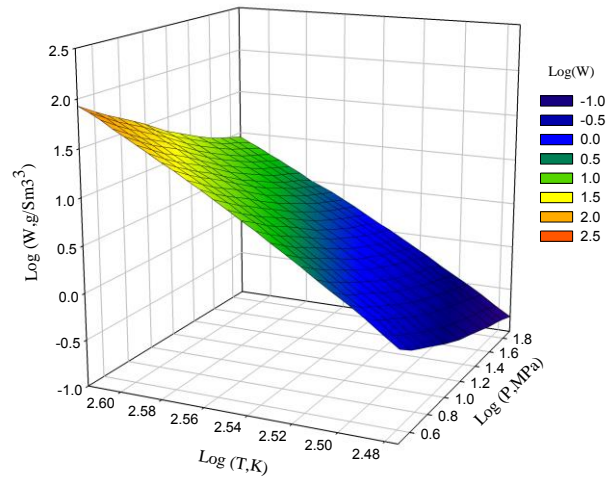


Figure 2 Representation of water content dependency on pressure and temperature in logarithmic form

3. Results and discussion

3. 1 New correlation parameters

In this step, all the gathered data should be used in a multi-dimension regression procedure. In order to find the parameters of correlation (7), available software such as Engineering Equation Solver (EES), Statistical Package for the Social Sciences (SPSS), and Polymath could be used. In this work, the Polymath has been employed for statistical analysis of the data.

Polymath allows the user to enter any linear or non-linear equation. This program uses the Levenberg-Marquardt (LM) algorithm for finding the parameter values, which minimize the sum of squares of the errors. The LM algorithm is an iterative technique that locates the minimum of a multivariate function that is expressed as the sum of squares of non-linear real-valued functions [23,26]. Detailed analysis of the LM can be found elsewhere [20,33, 34].

Error and sum of squares of deviations are defined by the following equations, respectively.

$$e_i = [\log(W)_i]_{\text{experimental}} - [\log(W)_i]_{\text{predicted}} \dots \quad (8)$$

$$S = \sum_{i=1}^n (e_i)^2 = \sum_{i=1}^n (\log(W)_i - A_1 \log(P) - \dots - B_1 \log(T) - \dots - C_1 \log(P) \times \log(T) - \dots - D) \quad (9)$$

In this method, the constants must be determined such that S is minimum. It is well known that the function S is a minimum when

$$\frac{\partial S}{\partial A_1} = \frac{\partial S}{\partial A_2} = \dots = \frac{\partial S}{\partial D} = 0 \quad (10)$$

To achieve more accurate results, the collected data are divided into two data sets based on pressure ranges. Obtained values for coefficients of correlation (7) are tabulated in Table 2.

Table 2 Tuned coefficients of new correlation

Constant	Pressure (MPa)	
	3-12.5	12.5-80
A_1	11.1728534218026	28.18757891000850
A_2	2.17088362926705	-4.412326505754120
A_3	-0.61245099784033	-0.110962892846461
B_1	613.998704849282	586.5149287949610
B_2	-217.137829772619	-204.8201385332070
B_3	26.01248692666940	24.44916368904060
C_1	-10.0477399537319	-16.18525794444430
C_2	-0.216589232258067	1.990971914315890
C_3	1.898617158773830	1.743708627795870
D	-583.2890363626920	-567.2953173754560

3. 2 New model in comparison with Ning *et al.* [32] correlation

Since both Ning *et al.* [32] and the proposed correlations are developed based on the McKetta - Wehe chart, first, the capability of these two models in predicting the water content of sweet natural gases have been compared. With the aim of checking the accuracy of these models in reproducing the extracted data from McKetta-Wehe chart, the absolute deviation (AD %) and average absolute deviation (AAD %) are used as statistical parameters.

$$AD\% = 100 \left| \frac{(W_{\text{exp}} - W_{\text{calc}})}{W_{\text{exp}}} \right| \dots \quad (11)$$

$$AAD\% = 100 \sum \left| \frac{(W_{\text{exp}} - W_{\text{calc}})}{W_{\text{exp}}} \right| / N \dots \quad (12)$$

where N is the number of the points.

The summary of obtained results from newly developed and Ning *et al.* [32] correlations for prediction of water content of sweet natural gases against the target data are presented

in Table 3. The graphical representation of Table (3) is depicted in Figure 3. *AD%* between the estimations of the new models and Ning *et al.* (2000) correlation and some data from McKetta - Wehe chart are given in Table 4. As it can be seen from error analysis results, the obtained mathematical model has overall *ADD %* equal to 0.86% while the Ning *et al.* [32] correlation showed absolute deviation in average 5.93%. So, the proposed model in this work covers the McKetta-Wehe chart more precisely than Ning *et al.* [32] correlation across all investigated ranges for pressure and temperature.

Table 3 Error analysis results for Ning *et al.* [22] and the new correlations

Pressure (MPa)	AAD %	
	New Correlation	Ning <i>et al.</i> [22]
3	0.73	4.94
4	0.97	9.35
5	0.79	11.86
6	0.90	4.96
8	0.71	6.70
10	1.33	5.91
15	0.86	4.77
20	0.81	4.67
30	0.67	4.37
40	0.97	4.23
50	0.72	3.56
60	0.85	5.12
80	0.86	6.56
Overall	0.86	5.93

Figure 3 Graphical representation of AAD % of Ning *et al.* [22] and the new correlation for various pressures

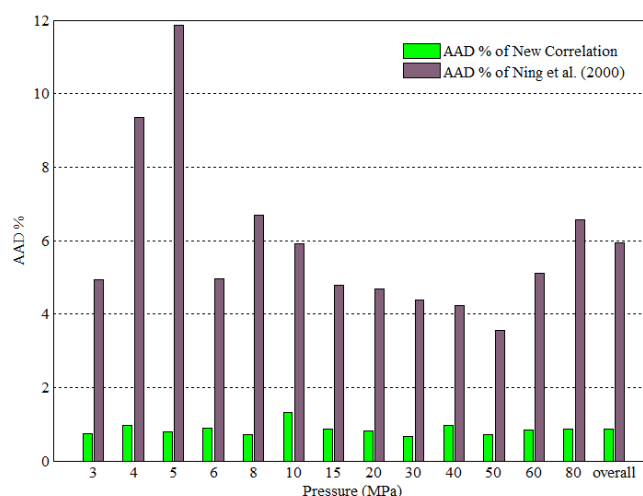


Table 4 The predictions of new and Ning *et al.* [22] correlations in comparison with some extracted data form McKetta-Wehe chart [20]

P (MPa)	T (K)	W (g/Sm ³)			AD%	
		Exp.	This work	Ning <i>et al.</i> [22]	This work	Ning <i>et al.</i> [22]
3	298.15	0.86556	0.86485	0.883581	0.082	2.082
3	358.15	14.0287	13.9983	14.32392	0.216	2.104
4	303.15	1.50474	1.51085	1.59306	0.406	5.869
4	368.15	15.8630	15.6465	17.2300	1.364	8.618
5	313.15	1.2905	1.28214	1.33580	0.646	3.511
5	383.15	21.5681	21.9707	25.8110	1.866	19.672
6	298.15	0.51871	0.51422	0.54389	0.866	4.855
6	378.15	16.0263	16.2645	17.4924	1.486	9.148
8	308.15	0.74231	0.73345	0.75536	1.194	1.757
8	403.15	29.3248	29.2184	32.4537	0.363	10.67
10	383.15	13.0582	13.3819	14.3807	2.479	10.13
10	413.15	32.4871	33.1589	35.6753	2.068	9.814
15	338.15	1.90439	1.90876	1.92539	0.229	1.103
15	398.15	14.9177	15.0436	16.0574	0.844	7.640
20	318.15	0.69807	0.69579	0.73037	0.326	4.627
20	408.15	16.5263	16.1485	17.3915	2.286	5.235
30	323.15	0.70526	0.71870	0.74825	1.906	6.096
30	373.15	4.5945	4.5069	4.55237	1.906	0.917
40	353.15	2.0044	2.0056	2.0019	0.056	0.126
40	408.15	10.531	10.608	11.243	0.727	6.758
50	368.15	3.0192	2.9866	2.9636	1.078	1.842
50	413.15	10.749	10.809	11.136	0.555	3.594
60	363.15	2.3613	2.3416	2.2819	0.834	3.363
60	398.15	6.7111	6.6818	6.6065	0.438	1.559
80	303.15	0.1901	0.1927	0.2299	1.333	20.92
80	413.15	8.8487	8.8163	9.1269	0.366	3.144

3.3. New model in comparison with other available methods

The approaches proposed by Bukacek [6], Chapoy [11] and Mohammadi *et al.* [29] for estimating the water content of natural gases have been chosen as a basis of comparison. In this section, the error analysis entails investigating the precision of the mentioned methods and the presented models against the previously published experimental data of natural gas water content in equilibrium with pure water.

Experimental data points of several systems include C_1 -water, C_2 -water, and C_1 - C_2 -water; have been collected from literature [10,39,36,41]. Table 5 shows the analysis of gathered data points.

Table 5 Sources of gathered experimental data along with data analysis summary

System	Ref.	N	Pressure, MPa		Temperature, K		$y_w \times 10^3$	
			min	max	min	max	min	max
C_1 -Water	[13]	25	5.99	34.61	298.11	318.12	0.265	1.985
	[39]	17	3.45	89.63	310.93	422.04	0.125	125
	[38]	12	4.23	14.37	310.93	344.26	0.754	9.33
C_2 -Water	[13]	12	3.24	4.63	293.11	303.11	0.525	1.41
	[39]	13	3.45	89.63	314.82	366.48	0.499	22.5
	[40]	15	2.76	13.79	310.93	344.26	0.812	12.69
C_1 - C_2 -Water	[38]	15	4.23	14.16	310.93	344.26	0.740	5.66
Overall	-	109	2.76	89.63	293.11	422.04	0.125	125

N denotes number of the points

Table 6 shows the performance of new correlation in comparison with other existing methods in regenerating the collected experimental data of C_1 -water, C_2 -water, C_1 - C_2 -water systems. Figure 4 demonstrate the performance evaluation in graphical form. More detailed comparison is provided in Appendix A.

Table 6 Summary of error analysis results for existing methods and new correlation

System	AAD %			
	This work	Bukacek [6]	Chapoy [13]	Mohammadi <i>et al.</i> [7]
C_1 -Water	4.20	4.45	10.46	4.58
C_2 -Water	8.68	12.38	8.64	10.10
C_1 - C_2 -Water	3.89	3.23	5.04	4.13
Overall	5.80	7.19	8.85	6.88

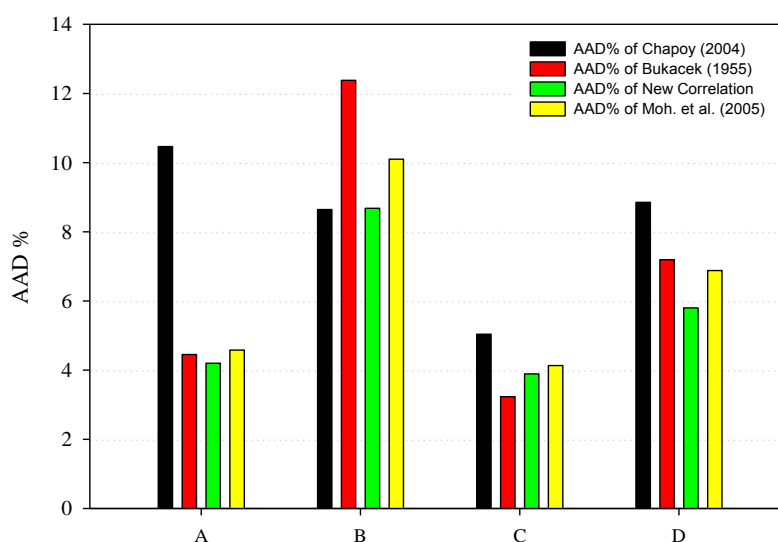


Figure 4 Graphical performance evaluation of existing methods and new correlation in reproducing collected experimental data (A, B, and C, denote C_1 -water, C_2 -water, and C_1 - C_2 -water systems, respectively, D stands for all gathered data)

As can be observed from Table 4 and also Figure 4, the overall performance of the proposed correlation in water content estimation is better than other existing methods. As mentioned before, none of the experimental data obtained from Sharma [39], Yarrison [41], Chapoy [10], and Reamer *et al.* [36] are employed in construction of the presented correlation. Regeneration of the experimental data with an AAD % of 5.80% corroborates good potency of the obtained empirical correlation in predicting water content of sweet natural gases.

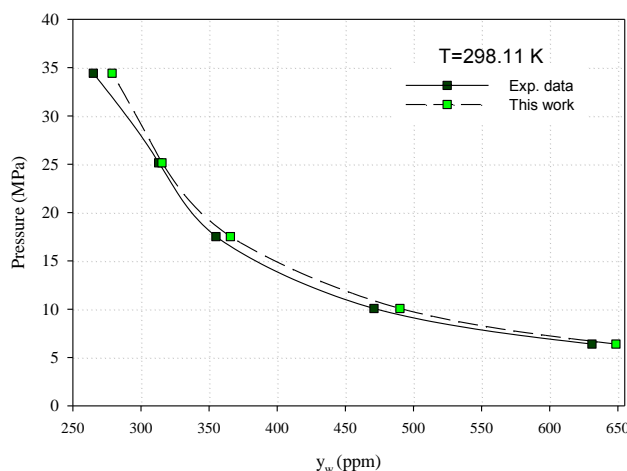


Figure 5 Experimental [13] and predicted water content of pure methane at 298.11 K

A comparison between the estimations of the new correlation and the experimental data published by Chapoy [10] for water content of pure methane at 298.11 K is illustrated in Figure 5. The Data reported by Yarrison [41] for pure ethane at 366.48 K, and the data reported by Sharma [39] for mixture of methane (91.73%) and ethane (8.27%) at 344.26 K along with the obtained results of new model are shown in Figures 6 and 7, respectively.

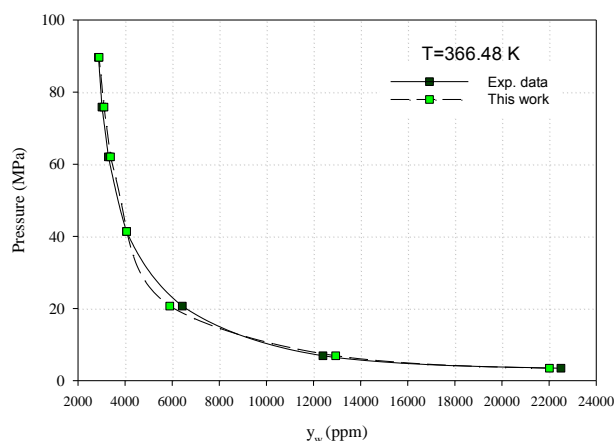


Figure 6 Experimental [39] and predicted water content of pure ethane at 366.48 K

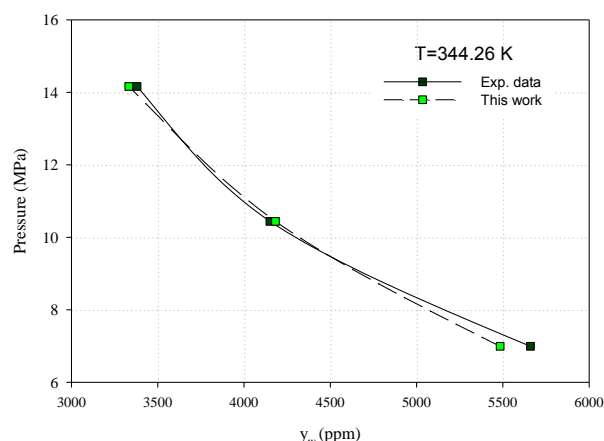


Figure 7 Experimental [38] and predicted water content of mixture of methane (91.73%) and ethane (8.27%) at 344.26 K

4. Summary and conclusions

In this study, a mathematical model in a polynomial form with 10 constants for fast and accurate estimation of sweet natural gas water content was presented. The required data for developing the correlation were gathered from McKetta -Wehe chart reproduced by GPSA [1]. The correlation is easy to use and is applicable for wide range of pressure (3-80 MPa) and temperature (298.15-413.15 K). New correlation showed absolute deviation in average

0.86%. Based on comparison results, the capability of proposed correlation in regenerating the data of McKetta-Wehe chart is much better than Ning *et al.* [32] correlation.

With the aim of performing further performance evaluation, some experimental data of the water content of pure methane, pure ethane, and mixtures of methane and ethane in equilibrium with pure water was collected from reliable sources [10,39,36,41]. It was demonstrated that the predictions of the new empirical model are in good agreement with experimental data.

Based on error analysis results, the obtained correlation is more accurate than the methods reported by Bukacek [6], Chapoy [10], and Mohammadi *et al.* [29] and can be used successively for prediction of sweet natural gas water content without considering sophisticated thermodynamic terms. In the case of sour or acid gases, the proposed correlation can be combined with appropriate approaches for calculation of water content of acid or sour gases. Such methods as Robinson *et al.* [37], Maddox *et al.* [25], and Bahadori *et al.* [4,5] rectify the sweet gas water content with regard to the amount of acid gases in the system. The obtained methods by Bahadori *et al.* [4,5] are more recommended, however, according to simplicity and excellent performance accompanied with those reported models.

List of symbols

a, A, A_i	Coefficient
AAD %	Average absolute deviation in percent
b, B, B_i	Coefficient
c, C_i	Coefficient
d, D	Coefficient
e_i	Deviation
EES	Engineering Equation Solver
LM	Levenberg-Marquardt
N	Number of points
P	Pressure (MPa)
p^{SAT}	Water vapor pressure
S	Sum of squares of deviations
SPSS	Statistical Package for the Social Sciences
T	Temperature (K)
W	Water content (g/Sm ³)
x_w	Mole fraction of water in liquid phase
y_w	Mole fraction of water in vapor phase

Greek symbols

ν_w^L	Water molar volume
ϕ_w	Fugacity coefficient of water in the gas phase

References

- [1] Aoyagi, K., Song, K. Y., Sloan, E. D., Dharmawardhana, P. B., Kobayashi, R., 1999. GPSA engineering data book, eleventh ed. Tulsa, OK: Gas Processors Suppliers Association and Gas Processors Association.
- [2] Bahadori, A., 2011a. Prediction of moisture content of natural gases using simple Arrhenius-type function. Cent. Eur. J. Eng. 1(1), 81-88.
- [3] Bahadori, A., 2011b. Novel predictive tools for oil, gas and chemical industries. VDM Verlag Publishing Company, Saarbrücken, Germany.
- [4] Bahadori, A., Vuthaluru, H. B., Mokhtab, S., 2009a. Method accurately predicts water content of natural gases, Energy Sources, Part A, 31, 754-760.
- [5] Bahadori, A., Vuthaluru, H. B., Mokhtab, S., 2009b. Rapid estimation of water content of sour natural gases. J. Jpn. Petrol. Inst., 52 (5), 270-274.
- [6] Bukacek, R.F., 1955. Equilibrium moisture content of natural gases. Institute of Gas Technology, Research Bulletin (8).
- [7] Burkill, J. G., 1959. Lectures on approximation by polynomials. Tata Institute of Fundamental Research, Bombay.
- [8] Carroll, J., 2009. Natural gas hydrates: A guide for engineers. Gulf Publishing Company, Burlington, USA.

- [9] Campbell, J. M., 1992. Gas conditioning and processing, Volume 1: The basic principles. seventh ed. Campbell Petroleum Series, Oklahoma, USA.
- [10] Chapoy, A., Haghighi, H., Burgass, R., Tohidi, B., 2010. Gas hydrates in low water content gases: Experimental measurements and modeling using the CPA equation of state. *Fluid Phase Equilib.* 296, 9–14.
- [11] Chapoy, A., 2004. Phase behaviour in water/hydrocarbon mixtures involved in gas production systems. PhD dissertation, Ecole Nationale Supérieure des Mines de Paris, Paris, France.
- [12] Daubert, T. E., Danner, R. P., 1985. DIPPR Data Compilation Tables of Properties of Pure Compounds, AIChE, New York, USA.
- [13] Erbar, J.H., Jagota, A.K., Muthswamy, S., Moshfeghian, M., 1980. Predicting synthetic gas and natural gas thermodynamic properties using a modified Soave Redlich-Kwong equation of state. GPA Research Report No. 42.
- [14] Gue, B., Ghalambor, A., 2005. Natural Gas Engineering Handbook. Gulf Publishing Company, Houston, Texas, USA.
- [15] Hoffman, J. D., 2001. Numerical methods for engineers and scientists, second ed. Marcel Dekker, Inc., New York, USA.
- [16] <http://www.mhhe.com/engcs/mech/ees/>.
- [17] <http://www.polymath-software.com>.
- [18] <http://www.spss.com>.
- [19] Jackson, D., 1934. A proof of Weierstrass's theorem. *The Am. Math. M.*, 41 (5), 309-312.
- [20] Kelley, C. T., 1999. Iterative methods for optimization. SIAM Press, Philadelphia, USA.
- [21] Kobayashi, R., Songand, K. Y., Sloan, E. D., 1987. Phase behavior of water/hydrocarbon systems. In: *Petroleum Engineers Handbook*, Bradley, H. B. (Ed.), Richardson, TX: Society of Petroleum Engineers.
- [22] Kohl, A., Nielsen, R., 1997. Gas Purification, fifth ed. Gulf Publishing Company, Houston, Texas, USA.
- [23] Levenberg, K., 1944. A method for the solution of certain non-linear problems in least squares. *Q. Appl. Math.* 2(2),164–168.
- [24] Li, Z., Firoozabadi, A., 2009. Cubic-plus-association equation of state for water-containing mixtures: Is "cross association" necessary?. *AIChE J.* 55 (7), 1803–1813.
- [25] Maddox, R. N., Lilly, L. L., Moshfeghian, M., Elizondo, E., 1988. Estimating water content of sour natural gas mixtures, Laurance Reid Gas Conditioning Conference, Norman, Oklahoma, USA, 8 March.
- [26] Marquardt, D. W., 1963. An algorithm for the least-squares estimation of nonlinear parameters. *SIAM J. of Appl. Math.* 11(2), 431-441.
- [27] McCain Jr., W.D., 1990. The properties of petroleum fluids, second ed. Pennwell Publishing Company, Tulsa, OK, USA.
- [28] McKetta, J. J., Wehe, A. H., 1958. Use this chart for water content of natural gases. *Petrol. Refin. (Hyd. Proc.)* 37, 153.
- [29] Mohammadi, A. H., Samieyan, V., Tohidi, B., 2005. Estimation of water content in sour gases. in: *SPE Europec/EAGE Annual Conference 2005*, Madrid, Spain, June 13-16, 2005.
- [30] Mohammadi, A. H., Chapoy, A., Tohidi, B., Richon, D., 2004. A semi-empirical approach for estimating the water content of natural gases. *Ind. Eng. Chem. Res.* 43 (22), 7137-7147.
- [31] Mokhatab, S., Poe, W. A., Speight, J. G., 2006. *Handbook of Natural Gas Transmission and Processing*. Gulf Publishing Company, Burlington, USA.
- [32] Ning, Y., Zhang, H., Zhou, G., 2000. Mathematical simulation and program for water content chart of natural gas. *Chem. Eng. Oil Gas.* 29, 75–77. In Chinese.
- [33] Nocedal, J., Wright, S. J., 1999. Numerical optimization. Springer Publishing Company, New York, USA.
- [34] Press, W. H., Teukolsky, S.A., Vetterling, A.W.T., Flannery, B.P., 1992. Numerical recipes in C: The art of scientific computing. Cambridge University Press, New York, USA.

- [35] Quarteroni, A., Sacco, R., Saleri, F., 2007. Numerical mathematics, second ed. Springer Publishing Company, Berlin, Heidelberg.
- [36] Reamer, H. H., Olds, R. H., Sage, B. H., Lacey, W. N., 1943. Phase equilibria in hydrocarbon systems, composition of a dew point gas in ethane-water system. *Ind. Eng. Chem.* 35, 790-793.
- [37] Robinson, J. N., Moore, R. G., Heidemann, R. A., Wichert, E., 1980. Estimation of the water content of sour natural gas, Laurance Reid Gas Conditioning Conference, Norman, Oklahoma, USA.
- [38] Robinson, J. N., Wichert, E., R. Moore, G., Heidemann, R. A., 1978. Charts help estimate H₂O content of sour gases. *Oil & Gas J.* 6 February, 76-78.
- [39] Sharma, S., 1969. Equilibrium water content of gaseous mixtures. PhD dissertation, The University of Oklahoma, Norman, Oklahoma, USA.
- [40] Wichert, G. C., Wichert, E., 2003. New charts provide accurate estimations for water content of sour natural gas. *Oil & Gas J.* 27 October, 64-66.
- [41] Yarrison, M., 2006. Measurement and modeling of the water content of high pressure sweet and acid natural gas systems. PhD dissertation, Rice University, Houston, Texas, USA.
- [42] Yang, W. Y., Cao, W., Chung, T. S., Morris, J., 2005. Applied numerical methods using Matlab. John Wiley & Sons, Inc., Publication, Hoboken, New Jersey, USA.
- [43] Zirrahi, M., Azin, R., Hassanzadeh, H., Moshfeghian, M., 2010. Prediction of water content of sour and acid gases. *Fluid Phase Equilib.* 299, 171-179.

Appendix A

Detail of comparison between experimental data and predictions from developed empirical correlation and existing methods

Mole fraction of water in vapor phase could be converted to water content by the following relation:

$$y_w = \frac{W}{760.4} \quad (\text{A.1})$$

AD %s between the experimental water content of C_1 -water, C_2 -water, C_1 - C_2 -water systems and the predictions of developed model and literature methods in water mole fraction are given in Tables (A.1) to (A.3), respectively.

Table A.1a Absolute deviation between the predictions of new correlation and other existing methods and the experimental water content (y_w = water mole fraction) of pure CH_4 from [13]

P (MPa)	T (K)	y_w $\times 10^3$	Absolute deviation (AD %)			
			This work	Bukacek [6]	Mohammadi <i>et al.</i> [7]	Chapoy [13]
6.39	298.11	0.631	2.79	7.92	2.04	0.02
10.07	298.11	0.471	4.05	6.18	6.39	0.03
17.52	298.11	0.355	2.98	3.25	10.31	11.45
6.06	303.11	0.889	0.89	4.70	3.14	1.51
9.84	303.11	0.625	4.18	5.94	4.48	1.23
17.50	303.11	0.456	3.84	3.86	***	12.97
5.99	308.11	1.114	3.72	9.85	3.08	4.65
9.84	308.11	0.807	4.65	6.17	2.46	2.89
6.06	313.12	1.516	2.35	3.47	1.77	0.33
9.98	313.12	1.045	2.98	4.29	2.60	2.43
17.47	313.12	0.715	0.56	8.11	***	18.70
4.02	318.12	1.985	4.24	1.77	2.32	1.01
10.01	318.12	1.326	3.22	4.44	0.98	3.69
17.50	318.12	0.890	1.25	9.57	***	20.66
25.15	298.11	0.313	0.78	0.39	***	39.20
34.42	298.11	0.265	5.21	4.87	***	***
25.06	303.11	0.371	9.56	7.96	***	48.45
34.56	303.11	0.331	7.79	6.96	***	***
17.49	308.11	0.577	5.29	5.21	***	15.09
25.09	308.11	0.495	4.68	2.98	***	39.76
34.58	308.11	0.447	1.39	0.29	***	***
25.17	313.12	0.626	4.58	2.85	***	37.76
34.61	313.12	0.575	0.67	1.92	***	***
25.12	318.12	0.763	7.75	6.05	***	39.45
34.61	318.12	0.691	3.32	1.96	***	***

Table A.1b Absolute deviation between the predictions of new correlation and other existing methods and the experimental water content (y_w = water mole fraction) of pure CH_4 from [38]

P (MPa)	T (K)	y_w $\times 10^3$	Absolute deviation (AD %)			
			This work	Bukacek [6]	Mohammadi <i>et al.</i> [7]	Chapoy [13]
4.23	310.93	1.882	9.74	0.69	4.89	4.54
6.99	310.93	1.341	9.83	6.15	11.87	9.87
10.44	310.93	0.919	1.95	3.26	4.37	1.33
13.89	310.93	0.754	2.12	5.18	2.95	7.86
4.23	327.59	4.3	11.48	1.47	3.25	2.92
6.99	327.59	2.79	3.84	0.61	1.99	0.31
10.44	327.59	1.93	6.79	7.89	4.79	9.20
14.37	327.59	1.71	3.51	1.74	4.05	3.61
4.23	344.26	9.33	15.90	5.45	5.59	5.31
6.99	344.26	5.5	0.28	5.00	4.85	6.14
10.44	344.26	4.25	1.59	0.46	0.12	2.53
13.89	344.26	3.68	8.18	6.18	4.90	0.87

Table A.1c Absolute deviation between the predictions of new correlation and other existing methods and the experimental water content (y_w = water mole fraction) of pure CH₄ from [39]

P (MPa)	T (K)	y_w X10 ³	Absolute deviation (AD %)			
			This work	Bukacek [6]	Mohammadi <i>et al.</i> [7]	Chapoy [13]
6.89	310.93	1.25	2.35	1.80	4.34	2.26
3.45	366.48	23.5	6.32	7.32	8.48	8.60
6.89	366.48	13.3	2.71	3.20	5.22	5.88
3.45	422.04	125	1.74	14.18	16.82	16.71
6.89	422.04	74.7	2.01	1.73	6.02	5.23
20.68	310.93	0.699	7.74	8.71	***	8.01
41.37	310.93	0.534	10.14	10.20	***	***
20.68	366.48	6.00	1.73	0.64	***	8.02
41.37	366.48	3.97	2.44	3.72	***	***
62.05	366.48	3.45	1.98	0.81	***	***
75.84	366.48	3.14	1.16	3.35	***	***
89.63	366.48	2.89	0.17	6.71	***	***
20.68	422.04	31.7	5.55	1.05	***	8.01
41.37	422.04	20.5	4.67	1.39	***	***
62.05	422.04	16.6	2.96	0.60	***	***
75.84	422.04	14.3	3.61	5.94	***	***
89.63	422.04	13.7	1.39	3.75	***	***

Table A.2a Absolute deviation between the predictions of new correlation and other existing methods and the experimental water content (y_w = water mole fraction) of pure C₂H₆ from [13]

P (MPa)	T (K)	y_w X10 ³	Absolute deviation (AD %)			
			This work	Bukacek [6]	Mohammadi <i>et al.</i> [7]	Chapoy [13]
3.24	293.11	0.66	20.34	31.61	23.06	19.95
3.32	293.11	0.626	24.25	35.99	26.97	23.81
3.48	293.11	0.595	25.65	37.64	28.14	25.05
3.75	293.11	0.525	34.09	46.80	36.02	32.93
3.53	298.11	0.982	0.27	10.18	3.70	1.21
3.99	298.11	0.794	12.53	23.26	15.23	12.74
4.01	298.11	0.768	15.90	26.92	18.62	16.06
4.12	298.11	0.749	16.44	27.33	18.82	16.33
3.37	303.11	1.41	4.22	5.60	0.62	1.86
4.38	303.11	0.99	10.91	21.11	13.99	11.74
4.48	303.11	0.943	14.54	24.86	17.39	15.14
4.63	303.11	0.911	15.81	25.88	18.15	15.99

Table A.2b Absolute deviation between the predictions of new correlation and other existing methods and the experimental water content (y_w = water mole fraction) of pure C₂H₆ from [39]

P (MPa)	T (K)	y_w X10 ³	Absolute deviation (AD %)			
			This work	Bukacek [6]	Mohammadi <i>et al.</i> [7]	Chapoy [13]
3.59	314.82	2.19	7.67	19.79	16.09	13.30
6.89	314.82	1.28	15.80	20.849	14.67	14.12
3.45	366.48	22.5	2.15	12.099	13.30	10.42
6.89	366.48	12.4	4.34	10.699	12.86	10.55
20.68	314.82	0.837	7.57	8.51	***	5.28
41.37	314.82	0.733	21.95	22.15	***	***
62.05	314.82	0.582	17.01	13.12	***	***
89.63	314.82	0.449	8.13	3.70	***	***
20.68	366.48	6.43	8.30	6.08	***	1.87
41.37	366.48	4.06	0.17	1.42	***	***
62.05	366.48	3.29	2.78	5.71	***	***
75.84	366.48	3.02	2.77	7.46	***	***
89.63	366.48	2.87	0.87	7.46	***	***

Table A.2c Absolute deviation between the predictions of new correlation and other existing methods and the experimental water content (y_w = water mole fraction) of pure C_2H_6 from [40]

P (MPa)	T (K)	y_w $\times 10^3$	Absolute deviation (AD %)			
			This work	Bukacek [6]	Mohammadi <i>et al.</i> [7]	Chapoy [13]
2.76	310.93	2.641	6.84	2.15	0.78	3.44
5.51	310.93	1.474	4.38	2.40	2.91	4.234
6.89	310.93	1.244	1.93	2.23	3.94	4.264
10.34	310.93	0.949	0.65	0.62	6.79	3.78
13.79	310.93	0.812	4.97	1.92	9.51	2.05
2.76	327.59	6.00	7.44	2.94	1.73	0.97
5.51	327.59	3.25	3.32	4.44	2.11	0.44
6.89	327.59	2.74	1.19	3.57	0.91	0.01
10.34	327.59	2.02	2.69	3.76	0.79	2.30
13.79	327.59	1.68	0.39	2.68	0.14	4.80
2.76	344.26	12.69	9.21	2.10	2.07	0.63
5.51	344.26	6.833	5.61	2.84	2.64	0.71
6.89	344.26	5.675	2.44	2.92	2.77	1.31
10.34	344.26	4.147	1.52	2.72	3.05	3.01
13.79	344.26	3.409	0.16	1.76	3.11	4.67

Table A.3 Absolute deviation between the predictions of new correlation and other existing methods and the experimental water content (y_w = water mole fraction) of C_1 - C_2 mixture from [38]

%C ₁	P (MPa)	T (K)	y_w $\times 10^3$	Absolute deviation (AD %)			
				This work	Bukacek [6]	Mohammadi <i>et al.</i> [7]	Chapoy [13]
91.73	4.23	310.93	1.892	10.21	1.21	5.38	5.10
	6.99	310.93	1.32	8.40	4.66	10.47	8.50
	10.44	310.93	0.924	1.40	2.70	4.89	0.71
	13.89	310.93	0.753	1.93	5.32	2.83	7.92
	10.44	327.59	2.225	7.36	6.42	9.10	5.34
	13.89	327.59	1.72	2.21	0.16	2.60	4.59
	6.99	344.26	5.66	3.10	2.03	1.88	3.06
	10.44	344.26	4.15	0.78	1.93	2.29	4.92
	14.16	344.26	3.38	1.42	0.78	2.26	6.67
	10.44	310.93	0.912	2.74	4.05	3.63	2.04
84.04	13.89	310.93	0.74	3.73	7.17	1.12	9.82
	10.44	327.59	2.23	7.58	6.63	9.31	5.56
	13.89	327.59	1.711	1.70	0.37	2.09	5.14
	10.44	344.26	4.17	0.30	1.44	1.80	4.42
	13.89	344.26	3.58	5.45	3.56	2.25	1.83