

IBP1581_11 A COMPARATIVE STUDY ON THE DIFFERENT ALTERNATIVES TO CALCULATE THE COMPRESSIBILITY FACTOR FOR NATURAL GAS Fábio Capelassi Gavazzi de Marco¹

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This Technical Paper was prepared for presentation at the *Rio Pipeline Conference & Exposition 2011*, held between September, 20-22, 2011, in Rio de Janeiro. This Technical Paper was selected for presentation by the Technical Committee of the event. The material as it is presented, does not necessarily represent Brazilian Petroleum, Gas and Biofuels Institute' opinion or that of its Members or Representatives. Authors consent to the publication of this Technical Paper in the *Rio Pipeline Conference & Exposition 2011.*

Abstract

It is well established the relevance of the compressibility factor on the analysis of the most diverse processes of oil and gas industry, from production to transport. Particularly in the transport of natural gas, its applicability takes place in many areas, some examples are: custody transfer, inventory estimations, leak detection, flow simulation, pipeline design, etc. Despite of all possible alternatives to calculate the compressibility factor the selection of a model requires special attention in order to have a good compromise between accuracy and complexity. Thus, the intent of this work is to present a critical evaluation about some options available to calculate the compressibility factor of natural gas and provide a starting point to support this choice. A large variety of equations of state and empirical correlations, totalizing seventeen, are analyzed under distinct scenarios comprised by lean and rich natural gas mixture with and without the presence of contaminants. The attention is concentrated on the envelope of pressure and temperature that is habitually found in the pipeline transport industry (0.1-20MPa and 270-370K). First, a set of experimental data is selected from different sources in the literature to identify the accuracy of the models and select the most accurate model. After that, a more comprehensive analysis is performed on the pressure-temperature envelope, considering the previously selected model as the reference. The Root Mean Square (RMS), Average Absolute Deviation (AAD), Systematic Deviation (BIAS), Standard Deviation (SD) and Deviation Span (DS) are presented for each model. As a general remark the results reveal that greatest source of discrepancy among the models has been a scenario where the rich natural gas without contaminant is considered.

1. Introduction

 One of the greatest challenges of oil and gas industry is the modeling the physical properties of its products and derivate. The natural gas is included within the class of fluid that requires an equation of state to represent its P-V-T relationship. In many situations, this comportment could be represented by ideal gas assumption, which is true in general, at low pressure and high temperature. However, most situations of practical interest in engineering, the real gas behavior is significantly far from the ideal one and would introduce a source of error in the results of an analysis.

 The correct determination of the natural gas compressibility factor and hence the density is fundamental in many process, Modisette (2000) emphasizes that is important in line-pack calculations, flow meter calibration, pressure drop calculations and compressor calculations. In the work of Chaczykowski (2009), is called attention to the selection of the Equation of State (EoS) on the sensitivity of pipeline gas flow model. Based on the EoS considered, the results suggest that the flow pattern and the pipeline line-pack are not significantly influenced by the EoS, on the other hand, leak detection models are highly sensitive by the EoS selection. Besides the application in engineering, the relevance of this subject in other fields is considerable, in the words of Wang et al. (2001): "The correct representation of the volumetric behavior of fluids in a wide range of pressure and temperature is recognized as one of the most important topics of applied thermodynamics".

 As is known there are innumerous possibilities to determine the behavior in terms of pressure, temperature and volume of a substance. This relationship is explained by an Equation of State (EoS) and according to Van Wylen et al. (1994) they could be categorized in three basic types: empirical, generalized and theoretical. Some traditional examples of empirical correlations are found in Annamalai and Puri (2002), like the well known EoS: Benedict–Webb–Rubin, Beatie–Bridgemann, Lee–Kesler and Martin–Hou, while, the EoS of van der Waals and Clasius are typically theoretical

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models. The empirical models rely on experimental observation of the fluids behavior, on the other hand, the theoretical models, arise from the molecular point of view of the fluids, like the kinetic theory of the gases or the Statistical Chain Theory, Avsec and Watanabe (2005). The generalized form, is the EoS expressed in terms of the reduced variables, pressure and temperature, that is supported by the theory of corresponding states. There is another classification of the EoS that is interesting under the scope of computational implementation and according to the relationship between the dependent and independent variables, it is classified as implicit and explicit. Obtaining the compressibility factor via an implicit EoS requires an iterative process of solution, and consequentially more processing effort is demanded, depending on the complexity of the model. Thus, the proper choice of an EoS should be guided by the range of pressure, temperature and gas composition with focus on the field of application. In spite of the vast amount of studies reported in literature addressing the accuracy of the equations of state, the present work is concerned with the transport of natural gas in pipelines.

2. Literature Review

 Traditionally the Standing and Katz (1942) chart has been the reference on the compressibility factor for natural gas. The chart is valid for hydrocarbon mixture only and does not consider the presence of contaminants. There are many works reporting the usage of these experimental data to compare models or develop new EoS.

The work of Wichert and Aziz (1971) present a comparison of twelve methods for determining the compressibility factor for natural gas containing H_2S and CO_2 . The model results are compared with experimental data considering six different types of natural gas mixture. The models were tested at a pressure ranging from 1.06 MPa to 48.44 MPa and a temperature range of 4.4°C to 148.9°C. The largest mean absolute error was attributed to the Benedict-Webb-Rubin equation (8.495%), while the smallest error was obtained by Robinson-Macrygeorgos-Govier method (1.031%). Although the Robinson-Macrygeorgos-Govier method has proved being accurate, it was not an attractive option because it is limited to a small range of pressure and temperature, and it is not suitable for computational use.

In the work of Al-Kamis (1995), nine EoS to predict the compressibility factor of the natural gas, including Leung, Papay, Papp and Burnett, have been evaluated. A total of 5940 experimental data points were taken from the Standing-Katz chart, and compared to the results of the correlations. The study comprises the range of application of reduced temperature varying from 1.05 to 3 and reduced pressure varying from 0.2 to 15. The results reveal the lowest absolute error, compared to original experimental data, and are given by Dranchuk and Abou-Kassem correlation, while the Hall and Yarborough correlation has given the lowest error, based on the experimental data with a correction introduced to smooth the curves of the reduced temperatures in 1.05 and 1.10.

Dranchuk et al. (1974) provided a new generalized EoS, based on the Benedict-Webb-Rubin. The equation has eight coefficients adjusted to the experimental data of the Standing-Katz chart. In Dranchuk et al. (1975), a similar procedure was employed to present an eleven coefficients equation. The authors verified that both equations have presented an average absolute error around 1 %, except in the vicinity of the critical point, where the error is around 60%.

Estela-Uribe and Trusler (2001) describe a procedure for obtaining some thermodynamic properties of the natural gas, including the compressibility factor. The idea presented is an extension of the concept of corresponding states, where an equation of state is used to obtain the properties of a reference fluid and from there extend to the gas mixtures. According to the authors, the average error of the method presented is slightly smaller than the error found by the procedure of AGA8.

Elsharkawy (2002) evaluates some methods for determining the compressibility factor, density and viscosity of natural gas containing N_2 , CO_2 and H_2S . The effect of incorporation of the binary interactions term on the ability of evaluating the gas properties by the equation of state is also studied. The author concluded that the Peng-Robinson had the best results near the critical region, while the EoS of Soave-Redlich-Kwong has a better accuracy in other combinations of temperature and pressure. However, the equation of state of Patel-Teja showed the best performance, especially when non-hydrocarbons are present in the mixture.

Estela-Uribe et al. (2003) present a virial EoS for calculating the natural gas properties specially developed for custody transfer. The mean absolute error in calculating the compressibility factor in the temperature range of 270K to 330K and pressure less than 12 MPa, was 0.034%.

Menon (2005) describe a very simple equation to calculate the compressibility factor of the natural gas, known as CNGA (California Natural Gas Association). The equation is explicit and the inputs are the reduced pressure and temperature and the gas specific gravity. The author claims the equation is valid for pressures greater than 689.5 kPa.

In the ISO 12213-2 (2006) presents the calculation procedure necessary for obtaining the compressibility of the natural gas via AGA8-92DC equation. The EoS employed in the detailed characterization method, known as AGA8-92DC is defined in as a hybrid because it combines traces of a virial-type equation, that is a power series in density, and traces of the Benedict-Webb-Rubin equation, that is the use of exponential function (Starling and Savidge, 1992).

Nasrifar e Bolland (2006) present a comparison of ten EoS, while one of them is proposed by the authors. The EoS are compared based on eight different natural gas mixtures. The cubic equation, presented by the author has given a error of 0.47%, while the other EoS under evaluation have given a minimum error of 0.81% and a maximum of 2.29%, using a set of 808 experimental data points.

Bahadori et al. (2007) have proposed an explicit correlation to the compressibility factor of the natural gas. The correlation takes into account the effect of carbon dioxide and hydrogen sulphide by means of a correction on the critical pressure and temperature. The authors also show a correlation to estimate pseudo-critical temperature and pressure as a function of the relative density of the gas.

In Al-Anazi and AlQuraishi (2010) an innovative concept is utilized to develop an EoS that is based on Genetic Programming technique. The authors have compared the proposed model and other ten models with experimental data, concluding that the proposed model has given the lowest average relative error, around 4%.

In Kamyab et al. (2010) it is proposed the use of neural network to obtain a correlation to calculate the compressibility of natural gases. The authors use the data of the Standing-Katz chart to develop two new explicit correlations. The models are compared to the Dranchuk and Abou-Kassem correlation (DAK), and the results report an average absolute error of 0.27%, 0.106% and 0.307%, respectively, for Kamyab5, Kamyab10 and DAK, using part of the experimental data as a reference.

Heindaryan et al. (2010) have presented an explicit correlation with ten constants. The constants of the equations have been obtained by least square regression of the experimental data of Standing-Katz chart and other additional experimental data. The experimental data comprise the range of reduced pressure from 0.2 to 15, while the reduced temperature is from 1.05 to 3. The authors do not recommend to use the equations for reduced temperature lower than 1.2.

2.1. Equations of State Evaluated

 Table 1 presents the EoS that are evaluated in this work, as well as, the year witch the model was conceived, the reference, the mixing rule used to calculate the natural gas properties and the characteristic of the equation.

EoS	Year	Reference	Mixing rule	Solution
Van der Waals	1873	Pedersen and Christensen (2007)	Van der Waals	Implicit
CNGA	1947	Menon (2005)	Kay	Explicit
Redlinch-Kwong	1949	Wichert e Aziz (1971)	Van der Waals	Implicit
Leung	1964	Al-Kahmis (1995)	Kay	Explicit
Papay	1968	Al-Kahmis (1995)	Kay	Explicit
Soave-Redlich-Kwong	1972	Bian et al. (1992)	Van der Waals	Implicit
Hall-Yarborough	1973	Kumar (2004)	Kay	Implicit
Dranchuk-Purvis-Robinson	1973	Dranchuk et al. (1974)	Kay	Implicit
Brill-Beggs	1974	Guo et al. (2007)	Kay	Explicit
Peng-Robinson	1976	Bian et al. (1992)	Van der Waals	Implicit
Papp	1979	Al-Kahmis (1995)	Kay	Explicit
Burnett	1979	Al-Kahmis (1995)	Kay	Explicit
AGA8-92DC	1992	ISO 12213-2 (2006)	Specific	Implicit
Bahadori	2007	Bahadori et al. (2007)	Kay	Explicit
Anazi	2010	Al-Anazi and Al-Quraishi (2010)	Kay	Explicit
Heidaryan	2010	Heidaryan et al. (2010)	Kay	Explicit
Kamyab10	2010 Kamyab et al. (2010)		Kay	Explicit

Table 1. Summary of the Equations of State under evaluation.

 Besides the mixing rule presented in the Table 1, the acentric factor employed in the Peng-Robinson and in the Soave-Redlich-Kwong equations has been calculated using the definition of Poling (2004).

3. Strategy of Evaluation

 The first part of this section describes the experimental references whereas the compressibility data have been collected to evaluate the variety of EoS. The second part is the hypothetical scenario that has been proposed to represent and cover the usual operation conditions found in the activities concerning the natural gas transport. In terms of natural gas pipeline the compressibility factor should be evaluated considering the possible variation of the natural gas composition within the envelope of operating pressures and temperatures that are typically found in this kind of process. The strategy adopted to evaluate the EoS is to perform a preliminary analysis using the experimental data and rank the results according to the definition detailed in the Statistical Analysis Section. After establishment of the EoS rank, by the comparison with experimental data, the EoS classified with the best rank is assumed as a reference to compare the remaining models throughout the hypothetical scenario analysis. As expected the data provided by the experimental references are limited, in terms of pressure, temperature and due to variation of the gas composition, thus, any conclusion based on this preliminary study would be incomplete.

3.1. Experimental Data

 As long as, the large amount of the EoS have been adjusted to a set of experimental data, that is traditionally the data taken form Standing Katz chart, considering these data again to evaluate the EoS would not lead to a consistent conclusion about the accuracy and how far from reality is the results given by a specific EoS. To avoid this, the experimental data of three distinct sources have been considered: Buxton and Campbell (1966), Li and Guo (1991) and Elsharkawy (2002). Those references do not consider the Standing-Katz data. Table 2 summarizes the range of pressure, temperature and composition of the data collected in the previously mentioned sources, where N is the number of experimental points that has been taken from the cited reference.

Reference	Z-Factor		Pressure (MPa)		Temperature (K)		Contaminant \mathscr{Y}_o		N
	Min	Max	Min	Max	Min	Max	Min	Max	
Buxton and	0.676	0.925	7.074	20.863	310.9	344.3	5.6	20.7	75
Campbell (1966)									
Li and Guo (1991)	0.883	0.993	0.662	7.534	310.2	358	0.7	174	47
Elsharkawy (2002)	0.719	0.969	4.826	22.753	209	219	0.7	71.6	10

Table 2. Range of the experimental data.

3.2. Hypothetical Scenario

 Despite of the evaluation that has been performed against the experimental data, it is necessary to check the EoS considering a complete range of pressure and temperature. Table 3 presents four possibilities for natural gas composition. These different mixtures are intended to represent the extreme situations regarding the natural gas quality. The four different mixtures are, lean and rich mixture with or without contaminants, where the molar fraction of each component of the mixture is defined in accordance with the limits established in the ANP-16 resolution (ANP, 2008).

Table 3. Molar fraction and critical properties of the natural gas mixtures.

 It was created a matrix of points to represent the envelope of operational condition usually found in the natural gas transport process, with pressure ranging from 0.1 MPa to 20 MPa and temperature ranging from 270K to 370K. The matrix has a resolution of 500x500, totalizing a hypothetical envelope of pressure and temperature with 250000 points. The intention is to perform a detailed survey on the ability of the EoS in corresponding to reality.

4. Statistical Analysis

In order to evaluate the differences originated in the diverse compressibility models a set of statistical parameters have been used. The criterions used in this work are defined in the Equations 1 thru 5, respectively, Root Mean Square (RMS), Average Absolute Deviation (AAD), Systematic Deviation (BIAS), Standard Deviation (SD) and Deviation Span (DS):

$$
BIAS = \frac{1}{N} \sum_{i=1}^{N} Z_i^{diff} \tag{1}
$$

$$
AAD = \frac{1}{N} \sum_{i=1}^{N} \left[\left(Z_i^{\text{diff}} \right)^2 \right]^{1/2} \tag{2}
$$

$$
SD = \left[\frac{1}{N-1} \sum_{i=1}^{N} \left(Z_i^{\text{diff}} - BIAS\right)^2\right]^{1/2} \tag{3}
$$

$$
RMS = \left[\frac{1}{N} \sum_{i=1}^{N} \left(Z_i^{\text{diff}}\right)^2\right]^{1/2} \tag{4}
$$

$$
DS = \left(Z_i^{\text{diff}}\right)_{\text{Maximum}} - \left(Z_i^{\text{diff}}\right)_{\text{Minimum}}
$$
\n(5)

where Z_i^{diff} is the Percent Relative Deviation, given by Equation 6:

$$
Z_i^{diff} = \frac{Z_i^{ref} - Z_i^{model}}{Z_i^{ref}} \cdot 100\%
$$
 (6)

 The rank is defined taking the average of RMS, AAD, SD, BIAS and DS, the best EoS is the one with the lowest average. Accordingly to Equation 7:

$$
Rank = \frac{1}{5} \left[\left(\frac{RMS}{RMS_{\text{max}}} \right) + \left(\frac{ADD}{ADD_{\text{max}}} \right) + \left(\frac{SD}{SD_{\text{max}}} \right) + \left(\frac{BIAS}{BIAS_{\text{max}}} \right) + \left(\frac{DS}{DS_{\text{max}}} \right) \right]
$$
(7)

5. Results

 The first part of this section is the comparison of the EoS with the experimental data that is presented in the Table 4. The classification of the EoS is based on the criteria established in the previous section. The rank is normalized, thus, the rank closer to one, means the model with the greatest deviation from experimental data among all models analyzed herein. The Papay model has received the rank 0.915, while the AGA8 model received the Rank 0.025, these are the extremes of the rank classification, and the first is the highest rank and consequentially is the EoS with the worst accuracy, based on the experimental data.

It should be emphasized that all the cubic EoS, except the VdW model, have agreed relatively well with the experimental set of dada considered herein, the greatest RMS error among these models has been placed below 2.35%, with the remaining parameters equally acceptable.

 Another important aspect that should be mentioned based on the results of Table 4 regards the variation in the results given by each model. Depending on the field of application, the variation bring in by the EoS in use would introduce a considerable error in final result of any study. Based on the innumerous possibilities available to calculate the compressibility of the natural gas, the models considered here are a small part of it. Thus, assuming this universe of possibilities is represented by the average results of Table 4, it is reasonable to assume that most of the processes involving the application of an EoS would have intrinsic error, in the worst case scenario would be around 18 %, that is the average deviation span of all models considered herein.

Table 4. Comparison with experimental data.

As long as the results of Table 4 have indicated the model with the lowest deviation compared to the experimental data, the next part of this work consider the AGA8 model as the reference and all the results are reported based on this reference. In the Figures 1 and 2 the RMS and DS are calculated for the mixtures of Table 3. It can be verified a trend regarding the magnitude of the deviation and the natural gas composition. The scenarios with rich natural gas have shown that in general the accuracy of the models is more sensitive to heavier hydrocarbons fractions in than the presence of contaminants in the composition.

Figure 1. RMS deviation, AGA8 as reference. Figure 2. Deviation span, AGA8 as reference.

 It should be mentioned that main purpose of the deviation span (DS) is to identify regions of localized discrepancy that would not be easily identified in the other statistical parameters, as has been identified in the Heidaryan model. This model in particular, have been failed to calculate the compressibility factor for pressure lower than 1 MPa, affecting significantly this statistical parameter, as shown in Figure 2.

 Table 5 gives the rank and the corresponding classification in parenthesis of each EoS according to criteria established in Equation 7 whereas the reference considered is the AGA8 model. The rank presented in Table 5 has been calculated using the different natural gas compositions of Table 3, with 250000 combinations of pressure and temperature for each model. Within the models with the lowest deviation, special attention should be given to the: Kamyab10, HY, Papp and Burnett models. As long as, these models are based on an explicit function it is expected that the associated computational effort is relatively small, they represented a good option as an EoS due to the compromise between accuracy and model complexity.

EoS	Lean	Rich	Lean $+$ Contaminant	$Rich +$ Contaminant	Average
VdW	0.133(13)	0.207(9)	0.143(11)	0.178(10)	0.165(10)
CNGA	0.116(11)	0.270(12)	0.380(14)	0.400(14)	0.292(13)
RK	0.030(2)	0.078(6)	0.028(1)	0.038(1)	0.043(1)
Leung	0.252(14)	0.324(14)	0.305(13)	0.337(13)	0.305(14)
Papay	0.920(16)	0.920(16)	0.925(14)	0.926(16)	0.923(16)
SRK	0.080(8)	0.118(7)	0.062(3)	0.075(8)	0.084(8)
HY	0.039(3)	0.033(1)	0.070(4)	0.053(2)	0.049(2)
DPR	0.131(12)	0.309(13)	0.142(10)	0.243(12)	0.206(12)
Brill-Beggs	0.044(5)	0.067(5)	0.079(8)	0.068(6)	0.065(6)
PR	0.064(7)	0.046(4)	0.070(5)	0.058(5)	0.059(4)
Papp	0.048(6)	0.042(3)	0.080(9)	0.073(7)	0.061(5)
Burnett	0.019(1)	0.189(8)	0.029(2)	0.055(4)	0.073(7)
Bahadori	0.104(10)	0.252(10)	0.161(12)	0.182(11)	0.175(11)
Ananzi	0.090(9)	0.257(11)	0.077(7)	0.153(9)	0.144(9)
Heidaryan	0.353(15)	0.403(15)	0.402(15)	0.413(15)	0.393(15)
Kamyab10	0.040(4)	0.035(2)	0.073(6)	0.054(3)	0.051(3)

Table 5. EoS rank and classification for each scenario.

 In the Figures 3 thru 10 are presented the AAD and SD calculated, respectively, according to Equation 2 and 3 and assuming the average among all the models as the reference. This analysis permits visualize the variations among the models and thus, identify the pressure and temperature combinations that is more prone to error. As indicated by the results, the upper left corner of the envelope, at low temperature and high pressure is the region of greatest divergence among the models. That is a clear trend that correlates well the magnitude of the deviation with the increase of the pressure, while the influence of the temperature has taken a secondary role.

Figure 3. Lean without contaminant (AAD %). Figure 4. Lean without contaminant (SD %).

Figure 7. Rich without contaminant (AAD %). Figure 8. Rich without contaminant (SD %).

Figure 9. Rich + Contaminant (AAD %). Figure 10. Rich + Contaminant (SD %).

Due to the large variety of options to calculate the natural gas compressibility factor, the engineers are free to decide and select the model that better attend the requirements for determined application. However, the liberty brought in by the diversity of EoS would lead to uncertainty in the situations where parts of a project are calculated with different EoS. Taking the example of the design and operation of a natural gas pipeline, if the design team make use of a EoS to determine the operational limits of the pipeline and operational team use another EoS to simulate the pressure

and temperature profiles, it is expected some divergences in the results. This perspective has been evidenced in the Figures 3 thru 10, as indicated the absolute deviation among the all models is about 12% in the worst case scenario, as well as the standard deviation is about 18%. Especially for the mixture rich without contaminant that has represented the situation with the highest deviations.

6. Conclusion

Based on the literate review and on the analysis performed in this work it was verified that is increasing the application of special numerical techniques in the development of new compressibility factor models. These techniques are seen especially in the works of Al-Anazi et al. (2010) and Kamyab et al. (2010), respectively, genetic programming and neural network. Both models are explicit functions, what implicates in less computational effort compared to the traditional EoS models, like PR, SRK, RK or AGA8. Moreover, the comparative analysis has demonstrated that the others models based on explicit functions have presented acceptable level of deviation from reference, like HY, Papp and Burnett models.

As a general remark there are some aspects especially important during the selection of an EoS. First is the more obvious and is regarded to the capability of the model in representing as close as possible the real behavior of the gas, in other words it is materialized in the global accuracy. The second aspect, concerns the standard deviations among the results of the various EoS in this study. It is very common in the gas industry practice to employ different EoS within the assortment of applications that require it. According to the application, the analysts prefer to choose a more accurate EoS or a simpler model. Per example in custody transfer, the AGA8 model is preferred, on the other hand, in the leak detection simulator the CNGA is a reasonable option due to computational efficiency. However, special attention should be given in the situation where there is exchange of information between these applications with different EoS. Thus, the analysis to indentify the absolute deviation and the standard deviation among all the models has been conducted, taking into account the pressure, temperature and composition range.

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