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Simplifying Hall-Yarborough Equation of State for Better Prediction of Hydrocarbon Compressibility Factors

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ABSTRACT— *This investigation demonstrates an advantage in the use of Pitzer's acentric factor as a third parameter in Hall-Yarborough equation of state for predicting gas compressibility factors. A simple modification has been introduced to parameter* Z_c *in the original Hall-Yarborough equation of state in terms of acentric factor* ω*, Critical Temperature* T_c*, and Critical Pressure* P_c*. This modified Hall-Yarborough equation is as simple as the Hall-Yarborough equation of state, yet achieves substantially better compressibility factor prediction accuracy of Hydrocarbons, especially at higher pressure. Results from the simplified Hall-Yarborough equation, the original Hall-Yarborough equation and practically obtained equation were compared with natural gas components data in a Dew point or retrograde gas condensate reservoir to demonstrate its accuracy and its application range. This new simple equation seems to be more accurate equation of state ever developed for non-polar and hydrocarbon systems and it greatly improves phase behavior studies of reservoir fluids.*

Keywords: — Acentric Factor, Compressibility Factor, Hall-Yarborough Equation, Dew Point/Retrograde Gas Reservoir, critical Deviation Factor, Newton/Raphson Iteration

1. INTRODUCTION

Gas utilization has become one of the primary goals of World's petroleum and energy policies. The role of natural gas in meeting the world energy demand has been increasing because of its abundance, versatility, and clean burning (Wang and Economides, 2009). Natural gas often contains some amounts of heavier hydrocarbon and non-hydrocarbon components that contribute to its properties. It is important to obtain accurate and reliable estimates of the physical properties of natural gas for optimal exploitation and usage. In most upstream and downstream petroleum and natural gas engineering calculations, the compressibility factor of natural gases are necessary to gas metering, gas compression, design of pipelines and surface facilities (Azizi et al. 2010). The natural gas compressibility factor is a measure of the amount of the gas deviate from perfect gas behavior. In gas industry, it is an important tool for computing reservoir fluid properties either directly or indirectly. The application of this important factor ranges:

evaluation of gas, gas flow in pipes, material balance calculations, well analysis, numerical reservoir simulations, etc. The common sources of Z-factor values are experimental measurements, equations of state (EOS) and empirical correlations. The most reliable and accurate way to obtain physical properties is from accurate experimental measurements. These experiments are expensive and time-consuming and it is impossible to measure properties for all possible compositions of natural gases (Ahmed, 2001). However, when laboratory analyses are not available, it is the task of empirical correlations and equations of state (EOS) to estimate the petroleum fluid properties as a function of the reservoir's readily available characteristics (Ahmed, 1989). Empirical correlations, which are used to predict natural gas Z-factor, are much easier and faster than equations of state. Sometimes these correlations have comparable accuracy to equations of state (Elsharkawy, 2004). In addition, equations of state (EOS) are more complex than the empirical correlations, involving a large number of parameters, which require more complicated and longer computations. This study presents a new simpler Hall-Yarborough equation of states for calculating gas compressibility factor based on acentric factor and mathematical modeling approach. Data for a variety of natural gases, covering lean, sweet to rich and acid or sour gases (H_2S, and CO_2) are collected from open literature. The proposed model efficiency is compared to two commonly used empirical correlations (Experimental formula and Hall-Yarborough equation of state) and several criteria are used to evaluate the developed model including the coefficient of determination (R^2), average relative error (ARE), average absolute relative error (AARE), and root mean square error (RMSE). In the following section, a review on some existing Z-factor estimation techniques is presented. Then, backgrounds of the proposed model and computation procedure are discussed in the subsequent sections. Accuracy and validation of the proposed models is checked later in Section 4. Subsequently, key findings of the present work are presented in Section 5.

Mathematically,

$$Z = f(T_r, P_r) \quad (1)$$

By definition,

$$P_r = \frac{P}{P_c} \quad (2)$$

$$T_r = \frac{T}{T_c} \quad (3)$$

Where P_c and T_c are critical pressure and critical temperature of the gas, respectively.

II. EQUATIONS OF STATE

Several forms of Equations of state (EOS) have been presented to the petroleum industry to calculate hydrocarbon reservoir fluid properties. Volumetric behavior is calculated by solving the cubic equation, usually expressed in terms of Z:

$$Z = \frac{PV}{RV} \quad (4)$$

$$Z^3 + A_2 Z + A_1 Z + A_0 \quad (5)$$

Where constants A_0, A_1, and A_2 are functions of pressure, temperature, and phase composition.

Empirical correlations: The lack of knowledge to calculate critical properties, acentric factors of plus-fraction's components and the binary interaction parameters involved in equations of state calculations resulted in utilization of empirical correlations which facilitated the computations and seemed to be more user-friendly models. This section presents a review of several widely used empirical correlations.

Gray-Sims method: This method involves the storage of a matrix composed of Z-values taken from the standing and Katz charts at some fixed values of pseudo reduced parameters P_r and T_r. An interpolation scheme is then used to compute deviation factors using the stored values. However, the range of applicability of this Z-factor calculation method is:

$$1.05 \leq T_r \leq 3.0$$

$$0.0 \leq Pr \leq 15.0$$

Sarem Method: The author made a least-square fittings of the Z= f (P_r, T_r) relationship using lagendre polynomials up to degree five. As a result of his work, only 36 coefficients were needed to be stored for calculating Z-factors. This made use of smaller-capacity mini-computers possible, a great achievement at that time. Range of applicability is

$$1.05 \leq T_r \leq 2.95$$

$$0.1 \leq P_r \leq 14.9$$

Carlie-Gillet Method: The Z-factors chart can be described by polynomials for the different pseudo reduced temperature of different degree, but not higher than 8. The coefficients were determined for different isotherms. Thus 17 linear equations must be written to produce the whole chart. Due to its large memory requirement, this method is impractical or even impossible on mini-computers. However, the ranges of its applicability are:

$$0.2 \leq T_r \leq 3.0$$

$$0.0 \leq P_r \leq 15.0$$

Hall-Yarborough method: This is an analytical approach to solving gas deviation-factor using starling-carnahan equation of state to develop the numerical model. Coefficients in the equation were determined by fitting it to the data taken from the Standing and Katz chart. Hall and Yarborough8 (1973) presented an equation-of-state that accurately determined the Standing and Katz z-factor chart. This is based on the Starling-Carnahan[21]equation-of-state. Best fit mathematical expressions were determined based on the data taken from Standing and Katz Z-factor chart. The mathematical form of the equation is:

$$Z = \left[\frac{0.06125 P_{pr} t}{Y}\right] EXP\left[-1.2(1-t)^2\right] \qquad (6)$$

Where P_{pr} = pseudo-reduced pressure.

t = reciprocal of the pseudo-reduced temperature = $\left[\frac{T_{pc}}{T}\right]$ (7)

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$$F(Y) = -0.06125P_{pr}\,te^{-1.2(1-t)^2} + \frac{Y + Y^2 + Y^3 - Y^4}{(1-Y)^3} - (14.76t - 9.76t^2 + 4.58t^3)Y^2 -$$

$$(90.7t - 242.2t^2 + 42.2t^3)Y^{(2.18+2.82t)} = 0 \quad (8)$$

The resulting non-linear equation can be solved for a function 'Y' using Newton-Raphson or secant iterative scheme. Here, Y is the reduced density which dependent on temperature. On programming the method to computer, storage requirement is small, making it suitable for mini-computers applications. The Newton-Raphson model provides easy converges in the range of applicability. Owing to its sound theoretical basis, this calculation method can be applied in a wider pseudo-reduced pressure range than the original chart. The authors using experimental data found out that it can give results of high accuracy even above P_r =24.0. The conservative limit of the correlation is:

$$1.2 \leq T_r \leq 3.0$$
$$0.1 \leq P_r \leq 24.0$$
$$1.05 \leq T_r \leq 3.0$$
$$0.2 \leq P_r \leq 30.0$$

Dranchuk and Kassem Method: These authors developed a method that adequately calculates Z-factor for pseudo-reduced temperatures lower than T_r =1.0. Their approach was similar to that of Hall-Yarborough in that they used the starling – carnahan equation of state. This method is valid in the range of:

$$1.0 \leq T_r \leq 3.0$$
$$2.0 \leq P_r \leq 30.0$$

Also for $P_r < 1.0$, and $0.7 < T_r \leq 1.0$. Beggs and Brill (1973) proposed a best-fit equation for the Standing and Katz z factor chart is as follows:

$$Z = A + \frac{(1-A)}{e^B} + CP_{pr}^D \quad (9)$$

Where

$$A = 1.39\left(T_{pr} - 0.92\right)^{0.5} - 0.36T_{pr} - 0.101 \quad (10)$$

$$B = \left(0.62 - 0.23T_{pr}\right)P_{pr} + \left[\frac{0.066}{\left(T_{pr} - 0.86\right)} - 0.037\right]P_{pr}^2 + \frac{0.32}{10^{9(T_{pr}-1)}}P_{pr}^6 \quad (11)$$

$$C = \left(0.132 - 0.32\log\left(T_{pr}\right)\right) \quad (12)$$

$$D = 10^{0.3106 - 0.49T_{pr} + 0.1824T_{pr}^2} \quad (13)$$

This method is cannot be used for reduced temperature (T_{pr}) values less than 0.92.

III. METHODOLOGY

P-V-T data were collected for twenty-one fluids studied in this investigation. These fluids ranged from non polar compounds like Hydrocarbon systems to strongly polar compounds. These different gas well composition were then computed into different natural gas properties using Microsoft excel environment. The computed gas properties are; T_c, P_c, P_{pr}, T_{pr}, apparent molecular weight, gas density, acentric factor etc, which were used for the development of new Z-factor correlation for Hydrocarbon systems to strongly polar compounds. In this method, acentric factor (ω) values were selected and regressed with corresponding critical compressibility factors

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(Z_c) values to give equations that expressed Z_c as a function of ω . This regression process had to be carried out for each acentric factor value. In a bid to ensure that the regression process gave rise to equations that were as accurate and reliable as possible, two regression exercises were carried out for each set of values. These two different exercises were carried out in such a way that they yielded two different equations – one linear and the other quadratic. Both equations expressed Z_c in terms of ω . The equations were of the form:

$$Z_c = A(\omega) + B \qquad (14)$$

$$Z_c = A(\omega)^2 + B(\omega) + C \qquad (15)$$

Where A, B, C are constants.

These two equations were subsequently tested over a range of values ω and the equation that gave z values were more in agreement with values obtained from the charts. In cases considered the linear equation proved more accurate than the quadratic equation. Table 1, 2 and figure1, 2 shows a summary of the regression analysis. Summary output for w and w^2.

Regression Statistics	
Multiple R	0.973250656
R Square	0.947216839
Adjusted R Square	0.944817604
Standard Error	0.006091485
Observations	24

ANOVA	df	SS	MS	F	Significance (F)
Regression	1	0.01464951	0.01464951	394.79959	1.52763E-15
Residual	22	0.000816336	3.71062E-05		
Total	23	0.015465846			

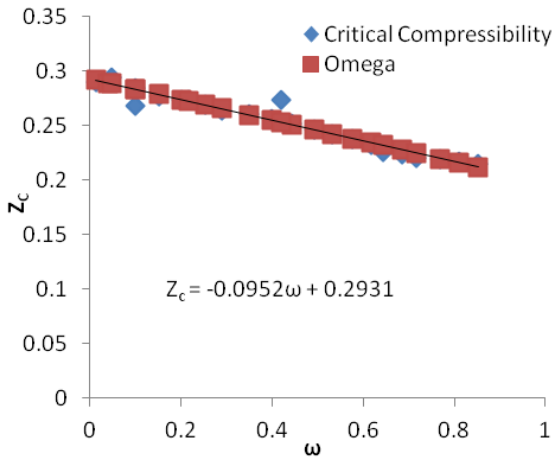

Fig 1: Plot of Z_c versus ω

Regression Statistics	
Multiple R	0.949610729
R Square	0.901760537
Adjusted R Square	0.897295107
Standard Error	0.008310334
Observations	24

ANOVA	df	SS	MS	F	Significance (F)
Regression	1	0.01394649	0.01394649	201.9426	1.45025E-12
Residual	22	0.001519356	6.9062E-05		
Total	23	0.015465846			

3.1 Technical Development

One of the most widely used and simple equation of state is the original Hall-Yarborough (OHY-EOS) given by the equation

$$Z = \frac{0.000660275\, t_r p_r z_c^{-3.6} \exp\left[-1.2\left(1-t_r\right)^2\right]}{y} \qquad (16)$$

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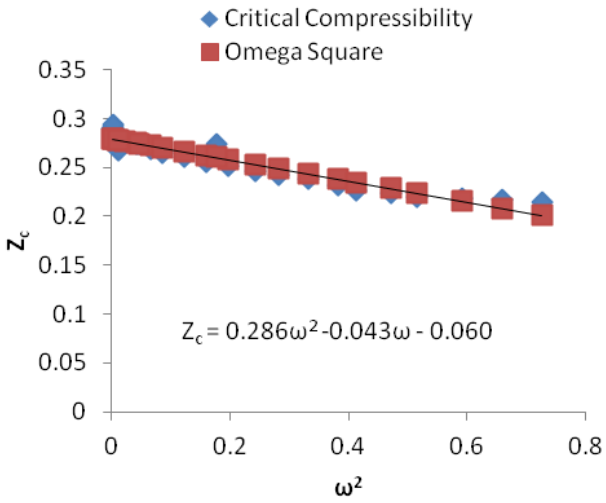

Fig 2: Plot of Z_c versus ω^2

The above equation Can now be written in terms of ω using the correlation between the critical deviation (Z_c) factor and the acentric factor (ω), as

$$Z_c = -0.0952\omega + 0.2931 \quad (17)$$

Substitute equation 17 into equation 16. Equation 16 changes to:

$$Z = \frac{0.000660275 t_r P_r (0.2931 - 0.0952\omega)^{-3.6} \exp\left[-1.2(1-t_r)^2\right]}{y} \quad (18)$$

Equation (18) becomes the operational equation from which the deviation factor can be obtained. Where t_r the reciprocal of pseudo-reduced temperature T_r and P_r is the reduced pressure. The objective function of the equation (18) above is to obtain the value of Z. To accomplish this, it is necessary to first determine the value of y, which is a reduced density term.

IV. RESULT AND DISCUSSION

Results obtained from the computer program were analyzed to ascertain their level of accuracy. In order to determine the accuracy of the simplified Hall-Yarborough equation of state, compressibility factor values obtained from simplified Hall-Yarborough equation of state, compressibility factor values obtained from the original Hall-Yarborough equation of state and compressibility factor obtained from experimental formular were compared in Table 3. A look at Table 3 as well as the plot (Fig 3) reveals that the results from this simplified Hall-Yarborough equation of state are actually more accurate and in harmony with those obtained from the original Hall-Yarborough equation of state and experimental equation. From table 3 which is a typical retrograde gas condensate reservoir, the model equation, achieved an absolute percentage difference of 2.1350% improvement over the original Hall – Yarborough. Here the result predicted by the modified equation agrees more closely with the experimental data especially at higher pressure than the value predicted by original hall – Yarborough. This might be responsible for the fairly large percentage difference of the experimental and the predicted values. However, since the reduced temperature (1.7) is within the validity range of the modified equation i.e. ($1.2 \leq T_r \leq 3.0$), a good prediction value was obtained. Even though an average improvement of 2.135% was made with the modified equation over the original Hall – Yarborough equation Fig 3 shows that at higher pressure especially at $P_r > 0.5$ the values predicted by the modified equation lies between the original Hall – Yarborough equation and the experimental values. This is

an indication of improvement of the modified equation over the original Hall – Yarborough equation which represent over estimated values and the laboratory values represent the under estimated values, the modified equation predicts the average of the two.

Table 3 Dew Point or Retrograde Gas Condensate Reservoir at P = 2700, and T = 180 °F

Nat Gas Comp	M. wt	Pr	tr	Z - EXP	Z – O.H.Y	Z- MOD	% Diff of Z Expand Z OHY	% Diff of Z Expand Mod
Pentadecane	212.42	12.582	1.991	0.726	1.722	1.596	-119.9	-137.3
Tetradecane	198.39	11.860	1.949	0.743	1.688	1.539	-107.1	-127.2
Tridecane	184.37	11.084	1.898	0.763	1.582	1.526	-100.0	-107.4
Dodecane	170.34	10.231	1.851	0.764	1.441	1.446	-89.32	-88.64
Undecane	156.31	9.554	1.797	0.777	1.387	1.384	-78.12	-78.46
Decane	142.29	8.825	1.737	0.783	1.306	1.328	-69.51	-66.75
Nonane	128.26	8.131	1.672	0.785	1.209	1.249	-59.23	-54.02
Octane	114.23	7.478	1.599	0.783	1.142	1.180	-50.65	-45.74
Heptane	100.2	6.796	1.519	0.768	1.040	1.086	-41.56	-35.55
Hexane	86.17	6.179	1.427	0.746	0.969	0.983	-31.66	-29.74
n-Pentane	72.15	5.526	1.321	0.706	0.941	0.887	-25.65	-33.34
i-pentane	72.15	5.506	1.295	0.709	0.851	0.867	-22.17	-19.99
Nitrogen	28.02	5.481	0.355	1.049	0.963	1.035	1.443	8.251
Carbonmonoxide	28.01	5.319	0.375	1.039	0.919	1.031	0.783	11.58
i-Butane	58.12	5.103	1.148	0.679	0.694	0.781	-14.99	-2.212
n-Butane	58.12	4.902	1.196	0.650	0.744	0.763	-17.31	-14.55
Propane	44.09	4.373	1.040	0.593	0.650	0.662	-11.63	-9.57
Methane	16.04	4.011	0.537	0.912	0.847	0.872	4.349	7.106
Ethane	30.07	3.795	0.859	0.568	0.562	0.598	-5.309	1.104
Benzene	78.11	3.779	1.582	0.408	0.465	0.491	-20.41	-13.95
Hydrogen sulfide	34.08	2.067	1.051	0.301	0.372	0.318	-5.429	-23.40
Avg. Abs % diff							2.130	2.110

This indicates that the model equation is accurate within the context of the original equation and very reliable, especially at higher pressure.

V. CONCLUSION

In this investigation work, Hall – Yarborough equation was modified to include critical compressibility factor in terms of the Pitzer acentric factor. The resulting equation was compared with the original Hall – Yarborough equation and with the

experimental equation. From all the plots of the three equations, we see that the curves followed an expected characteristic shape of gas deviation factor. This is a good indication that the model equation is correct. The critical deviation factor used by Hall – Yarborough in their original equation is a fixed value, which does not give room for any flexibility.

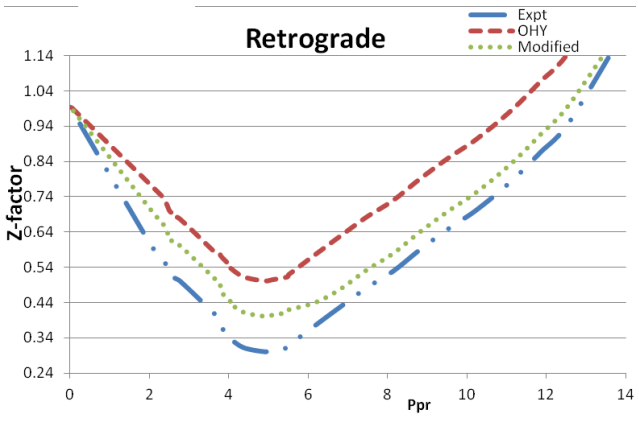

Fig 3: Shows a comparison of the three model equations in a typical retrograde gas condensate reservoir

The values predicted by the modified equation always lies between the values predicted by the original Hall – Yarborough and the values of the experimental data at higher pressure especially at $P_r > 0.5$. In conclusion, we can state as follows:

(a) Acentric factor is a good correction factor for size and shape effect of molecules.

(b) Inclusion of critical deviation factor in the prediction equation shows significant improvement.

(c) The modified Hall – Yarborough (model) equation is recommended for the prediction of complex fluid deviation factor covering the range of gas production, processing and transmission for $P_r \leq 25$ and $1.2 \leq T_r \leq 3.0$.

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Nomenclature	
Ω	– Acentric factor
Υ	– Gas specific gravity
Z_c	– Critical compressibility factor
P_c	– Critical pressure, Psi
T_c	– Critical temperature, ^oR
Y	– Reciprocal of gas density, ft^3/lb-m
Ppr	– Pseudo reduced pressure
T_{tr}	– Pseudo reduced temperature
Z	– Gas compressibility factor
ρ_g	– Gas density