Rapidly Estimating Natural Gas Compressibility Factor

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Abstract: Natural gases containing sour components exhibit different gas compressibility factor ($Z$) behavior than do sweet gases. Therefore, a new accurate method should be developed to account for these differences. Several methods are available today for calculating the $Z$-factor from an equation of state. However, these equations are more complex than the foregoing correlations, involving a large number of parameters, which require more complicated and longer computations. The aim of this study is to develop a simplified calculation method for a rapid estimating $Z$-factor for sour natural gases containing as much as 90\% total acid gas. In this article, two new correlations are first presented for calculating the pseudo-critical pressure and temperature of the gas mixture as a function of the gas specific gravity. Then, a simple correlation on the basis of the standard gas compressibility factor chart is introduced for a quick estimation of sweet gases’ compressibility factor as a function of reduced pressure and temperature. Finally, a new corrective term related to the mole fractions of carbon dioxide and hydrogen sulfide is developed.

Key words: natural gas; compressibility factor; sour gas; critical pressure; critical temperature

1. Introduction

The volume of a real gas is usually less than that of an ideal gas, and hence a real gas is said to be supercompressible. The ratio of the real volume to the ideal volume, which is a measure of the amount the gas deviates from perfect behavior, is called the supercompressibility factor, sometimes shortened to the compressibility factor. It is also called the gas deviation factor and is denoted by the symbol $Z$. The gas deviation factor is, by definition, the ratio of the volume actually occupied by a gas at a given pressure and temperature to the volume it would occupy if it behaved ideally.

The real gas equation of state is then written as

$$PV = ZnRT$$

where $P$ is the pressure, $V$ is the volume, $T$ is the absolute temperature, $Z$ is the compressibility factor, $n$ is the number of kilomoles of the gas, and $R$ is the gas constant.

The gas deviation factor, $Z$, is close to 1 at low pressure and high temperature, which means that the gas behaves as an ideal gas in these conditions. At standard or atmospheric conditions the gas $Z$ factor is always approximately 1.

The most common sources of $Z$-factor values are experimental measurement, equations-of-state method and empirical correlations. Necessity arises when there is no available experimental data for the required composition, pressure, and temperature conditions. Several different correlations are available for this important parameter. The basic correlations use the corresponding states concept.

The theory of corresponding states dictates that the $Z$ factor can be uniquely defined as a function of reduced pressure and reduced temperature. The reduced pressure and reduced temperature are defined

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as

\[ P_r = \frac{P}{P_c} \] (2)

\[ T_r = \frac{T}{T_c} \] (3)

where \( P_r \) and \( T_r \) are reduced pressure and reduced temperature, respectively, and \( P_c \) and \( T_c \) are critical pressure and critical temperature of the gas, respectively. The values of critical pressure and critical temperature can be estimated from the following equations if the composition of the gas and the critical properties of the individual components are known:

\[ P_c = \sum_{i=1}^{n} P_{ci}y_i \] (4)

\[ T_c = \sum_{i=1}^{n} T_{ci}y_i \] (5)

where \( P_{ci} \) and \( T_{ci} \) are the critical pressure and critical temperature of component \( i \), respectively; and \( y_i \) is the mole fraction of component \( i \).

Once the critical properties of the mixture are calculated as stated in Equations (4) and (5), we can use Equations (2) and (3) to calculate the reduced properties of the mixture.

If the gas compositions are known, several methods are available today for calculating the compressibility factor from an equation of state. Simultaneously, specific empirical methods have been developed, on the initiative of the gas companies, to calculate the compressibility factor of a commercial natural gas, particularly the AGA8 method developed in the United States by the Gas Research Institute-GRI [1] and the GERG method developed in Europe by a group of European gas companies [2]. However, these equations require more complicated and longer computations [3]. Numerous methods have been suggested to predict the pseudo-critical properties of the gases as a function of their specific gravity. The point to be noted here is that these methods predict the pseudo-critical values which are evidently not accurate values of the gas mixtures. The existing methods fail to predict the accurate values of pseudo-critical values when non-hydrocarbon components are present in significant amounts.

2. New proposed correlations

In this article, new equations are developed on the basis of SI units for gas compressibility factor of natural gases (\( Z \)), prediction of critical temperature \( (T_c) \) and critical pressure \( (P_c) \) of natural gases and sour gas compressibility correction. The experimental data to develop \( T_c \) and \( P_c \) prediction have been used from Sutton’s work, for gas compressibility factor the Standing-Katz chart [4] data were used to develop “\( Z \)” factor correction, and Wichert-Aziz [5] reported data have been used to develop sour gas correction correlation.

The values of critical pressure and critical temperature can be estimated from its specific gravity if the composition of the gas and the critical properties of the individual components are not known. Considering this, in this study, we used a regression analysis on the experimental data compiled by Sutton [6] to obtain the following second-order fits for the pseudo-critical properties:

\[ K = A_1 + B_1 \gamma_g + C_1 \gamma_g^2 \] (6)

In the aforementioned equation, parameter \( K \) is defined in Table 1, where \( P_{pc} \) and \( T_{pc} \) are pseudo-critical pressure (kPa) and pseudo-critical temperature (K), respectively, and \( \gamma_g \) is the specific gravity of gas. Equation (6) is valid over the range of specific gas gravities: \( 0.55 < \gamma_g < 1.75 \).

<table>
<thead>
<tr>
<th>( K )</th>
<th>( P_{pc} ) (kPa)</th>
<th>( T_{pc} ) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_1 )</td>
<td>5.216514285E3</td>
<td>9.3816666E1</td>
</tr>
<tr>
<td>( B_1 )</td>
<td>-9.0296428E2</td>
<td>1.9416666E2</td>
</tr>
<tr>
<td>( C_1 )</td>
<td>-2.4814285E1</td>
<td>-4.111111E1</td>
</tr>
</tbody>
</table>

The most commonly used method to estimate the \( Z \) factor is the chart provided by Standing and Katz [4]. The chart covers the range of reduced pressure from 0 to 15, and the range of reduced temperature from 1.05 to 3. For this reason, a Standing and Katz [4] curve regression analysis was used to determine four coefficients that correlate the gas compressibility factor, reduced pressure, and reduced temperature.

Therefore, the following approach is repeated for predicting the tuned coefficients reported in Table 2.

1 — Select reduced temperature form Standing-Katz chart.

2 — Select reduced pressures from Standing Katz chart.

3 — Correlate compressibility factor as a function of reduced pressure at a constant reduced temperature from Standing-Katz chart.

4 — Repeat steps 2 and 3 for other data at other reduced temperatures.
5 — Correlate corresponding polynomial coefficients which were obtained in previous steps as a function of reduced temperatures, \(a = f(T_r)\), \(b = f(T_r)\), \(c = f(T_r)\), \(d = f(T_r)\) it means Equations (8)–(11).

6 — Repeat steps 1 to 5 for other data.

7 — Calculate \(Z\) as a function of reduced pressure from Equation (7).

\[
Z = a + bP_{pr} + cP_{pr}^2 + dP_{pr}^3
\]

where

\[
a = A_a + B_aT_{pr} + C_aT_{pr}^2 + D_aT_{pr}^3
\]

\[
b = A_b + B_bT_{pr} + C_bT_{pr}^2 + D_bT_{pr}^3
\]

\[
c = A_c + B_cT_{pr} + C_cT_{pr}^2 + D_cT_{pr}^3
\]

\[
d = A_d + B_dT_{pr} + C_dT_{pr}^2 + D_dT_{pr}^3
\]

The tuned coefficients in Equations (8)–(11) are given in Table 2. Equation 7 has been presented to estimate the sweet gases compressibility factor over the range of \(0.2 < P_{pr} < 16\) and \(1.05 < T_{pr} < 2.4\). The advantage of Equations (7)–(11) is that it is explicit in \(Z\) and thus does not require an iterative solution as is required by other methods, such as that of the widely used equations of Dranchuk and Abou-Kassem [7]. Equations (7)–(11) also follow the cubic equation approach that has been widely applied to equations of state models.

Table 2. Tuned coefficients used in Equations (8)–(11)

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Tuned coefficients for gas compressibility factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A_a)</td>
<td>0.969469</td>
</tr>
<tr>
<td>(B_a)</td>
<td>-1.349238</td>
</tr>
<tr>
<td>(C_a)</td>
<td>1.443959</td>
</tr>
<tr>
<td>(D_a)</td>
<td>-0.36860</td>
</tr>
<tr>
<td>(A_b)</td>
<td>-0.107783</td>
</tr>
<tr>
<td>(B_b)</td>
<td>-0.127013</td>
</tr>
<tr>
<td>(C_b)</td>
<td>0.100828</td>
</tr>
<tr>
<td>(D_b)</td>
<td>-0.012319</td>
</tr>
<tr>
<td>(A_c)</td>
<td>0.0184810</td>
</tr>
<tr>
<td>(B_c)</td>
<td>0.0523405</td>
</tr>
<tr>
<td>(C_c)</td>
<td>-0.050688</td>
</tr>
<tr>
<td>(D_c)</td>
<td>0.010870</td>
</tr>
<tr>
<td>(A_d)</td>
<td>-0.000584</td>
</tr>
<tr>
<td>(B_d)</td>
<td>-0.002146</td>
</tr>
<tr>
<td>(C_d)</td>
<td>0.0020961</td>
</tr>
<tr>
<td>(D_d)</td>
<td>-0.000459</td>
</tr>
</tbody>
</table>

The \(Z\) factor chart of Standing and Katz [4] is only valid for mixtures of hydrocarbon gases. Wichert and Aziz [5] had previously compiled measured data for hydrocarbon gases that included acid gases and developed a correlation to fit the data. Their correlation was based on a power law fit that was not consistent with cubic EOS models. For this reason, we developed a cubic correlation to account for the inaccuracies in the Standing and Katz chart when the gas contains significant fractions of acid gases, specifically carbon dioxide (CO\(_2\)) and hydrocarbon sulfide (H\(_2\)S). Once the modified pseudo-critical properties are obtained, they are used to calculate pseudo-reduced properties and the \(Z\) factor is determined from Equation (7). The new correlation first calculates a deviation parameter \(\varepsilon\):

\[
\varepsilon = \frac{a + b y_{H_2S} + c y_{CO_2}^2 + d y_{H_2S}^3}{1.8}
\]

where

\[
a = A_a + B_a y_{CO_2} + C_a y_{CO_2}^2 + D_a y_{CO_2}^3
\]

\[
b = A_b + B_b y_{CO_2} + C_b y_{CO_2}^2 + D_b y_{CO_2}^3
\]

\[
c = A_c + B_c y_{CO_2} + C_c y_{CO_2}^2 + D_c y_{CO_2}^3
\]

\[
d = A_d + B_d y_{CO_2} + C_d y_{CO_2}^2 + D_d y_{CO_2}^3
\]

where, \(y_{H_2S}\) and \(y_{CO_2}\) are the mole fractions of H\(_2\)S and CO\(_2\) in the gas mixture, respectively. The tuned coefficients used in Equations (13)–(16) are also given in Table 3. These tuned coefficients help to cover sour natural gases up to as much as 90% total acid gas. These tuned coefficients are changed if more

Table 3. Tuned coefficients used in Equations (13)–(16)

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Tuned coefficients for critical temperature and pressure adjustment factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A_a)</td>
<td>4.094086</td>
</tr>
<tr>
<td>(B_a)</td>
<td>1.15680575E2</td>
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<tr>
<td>(C_a)</td>
<td>-1.6991417E2</td>
</tr>
<tr>
<td>(D_a)</td>
<td>5.62209803E1</td>
</tr>
<tr>
<td>(A_b)</td>
<td>1.45517461E2</td>
</tr>
<tr>
<td>(B_b)</td>
<td>-3.9672762E2</td>
</tr>
<tr>
<td>(C_b)</td>
<td>3.93741592E2</td>
</tr>
<tr>
<td>(D_b)</td>
<td>-2.17915813E2</td>
</tr>
<tr>
<td>(A_c)</td>
<td>-1.95766763E2</td>
</tr>
<tr>
<td>(B_c)</td>
<td>3.835331543E2</td>
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<tr>
<td>(C_c)</td>
<td>-6.08818159E2</td>
</tr>
<tr>
<td>(D_c)</td>
<td>3.704173461E2</td>
</tr>
<tr>
<td>(A_d)</td>
<td>5.24425341E1</td>
</tr>
<tr>
<td>(B_d)</td>
<td>-2.0133960E2</td>
</tr>
<tr>
<td>(C_d)</td>
<td>3.51359351E2</td>
</tr>
<tr>
<td>(D_d)</td>
<td>-2.20884255E2</td>
</tr>
</tbody>
</table>
accurate experimental data are available by proposed numerical model.

Then, \( \varepsilon \) is used to determine the modified pseudo-critical properties as follows:

\[
T_{pc}^{\text{correct}} = T_{pc} - \varepsilon \tag{17}
\]

\[
P_{pc}^{\text{correct}} = \frac{P_{pc}(T_{pc} - \varepsilon)}{T_{pc} + \varepsilon y_{H_2S}(1 - y_{H_2S})} \tag{18}
\]

Equation (12) is applicable to concentrations of \( \text{CO}_2 < 55 \text{ mol}\% \) and \( \text{H}_2\text{S} < 75 \text{ mol}\%, and has an average absolute error of 1\% over the following ranges of data: 1000 kPa < \( P < 45000 \text{ kPa} \), and 275 K < \( T < 425 \text{ K} \).

3. Case study

In this case example, we calculate the \( Z \) factor for a gas with the following properties and conditions (\( \gamma_g = 0.7, \text{H}_2\text{S}=7\% \) and \( \text{CO}_2=10\% \), \( P=13860 \text{ kPa} \) and \( T=297 \text{ K} \)) using our new proposed method and then compare it with the value obtained from Wichert and Aziz [5] correlation.

The process for the calculation is as follows:

First calculate the pseudo-critical properties:


\[
P_{pc} = 756.8 - 131.07\gamma_g - 3.6\gamma_g^2 = 4574 \text{ kPa}
\]

\[
T_{pc} = 169.2 + 349.5\gamma_g^2 - 74.0\gamma_g^2 = 210 \text{ K}
\]

From Equation 6:

\[
P_{pc} = 4572.28 \text{ kPa} \quad \text{and} \quad T_{pc} = 209.59 \text{ K}
\]

Next, calculate the adjustments to the pseudo-critical properties:

Using Wichert and Aziz [5] correlation (after unit conversion to SI):

\[
\varepsilon = 120(A^{0.9} - A^{1.6}) + 15(B^{0.5} - B^4)
\]

where \( A \) is the sum of the mole fractions of \( \text{CO}_2 \) and \( \text{H}_2\text{S} \) in the gas mixture and \( B \) is the mole fraction of \( \text{H}_2\text{S} \) in the gas mixture.

\[
\varepsilon = 120(0.17^{0.9} - 0.17^{1.6}) + 15(0.07^{0.5} - 0.07^4)
\]

\[
= 11.8 \text{ K}
\]

Then, using Equations (17) and (18), \( T'_{pc} = 196.3 \text{ K} \) and \( P'_{pc} = 4330 \text{ kPa} \).

From Equations (12)–(18): \( \varepsilon = 11.612 \text{ K} \); \( T'_{pc} = 197.98 \text{ K} \); \( P'_{pc} = 4287.73 \text{ kPa} \).

Finally, after calculating the pseudo-reduced properties, the \( Z \) factor will be \( Z = 0.772 \) from Standing and Katz [4] chart; \( Z = 0.7689 \) from Equation (7).

As can be seen from this example, the values predicted by the proposed correlations have good agreement with the calculated results by Wichert and Aziz [5] correlation. Thus, the proposed simple-to-use method is recommended for a rapid estimation of gas compressibility factor.

4. Results

Figures 1 and 2 illustrate the results of the new presented correlations for predicting the pseudo-critical temperature and pseudo-critical pressure as a function of gas specific gravity.

![Figure 1. Predicting pseudo-critical temperature using the new proposed equation](image1)

![Figure 2. Predicting pseudo-critical pressure using the new proposed equation](image2)
routine correlations. The advantage of the proposed correlation is that it is explicit in $Z$ and thus does not require an iterative solution as is required by other methods. The source of data to correlate these new correlations are from References 4, 5, and 6.

**Figure 3. Determining the critical temperature and pressure adjustment factor using new developed correlation**

(1) CO$_2$ mole fraction=0.85, (2) CO$_2$ mole fraction=0.80, (3) CO$_2$ mole fraction=0.75, (4) CO$_2$ mole fraction=0.65, (5) CO$_2$ mole fraction=0.60, (6) CO$_2$ mole fraction=0.55, (7) CO$_2$ mole fraction=0.50, (8) CO$_2$ mole fraction=0.45, (9) CO$_2$ mole fraction=0.40, (10) CO$_2$ mole fraction=0.35, (11) CO$_2$ mole fraction=0.30, (12) CO$_2$ mole fraction=0.25, (13) CO$_2$ mole fraction=0.20, (14) CO$_2$ mole fraction=0.15, (15) CO$_2$ mole fraction=0.10, (16) CO$_2$ mole fraction=0.05

**5. Conclusions**

In this article, a simplified calculation method for a rapid estimation of the $Z$-factor for sour natural gases containing as much as 90% total acid gas is studied. Two new correlations are first presented for calculating the pseudo-critical pressure and pseudo-critical temperature of the gas mixture as a function of the gas specific gravity. Then, a simple correlation based on the standard gas compressibility factor chart is introduced for a quick estimation of sweet gases’ compressibility factor as a function of reduced pressure and reduced temperature. Finally, a new corrective term related to the mole fractions of carbon dioxide and hydrogen sulfide is developed. The advantage of the proposed correlation is that it is explicit in $Z$ and thus does not require an iterative solution as is required by other methods.

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**Nomenclature**

$A$ — tuning coefficient
$B$ — tuning coefficient
$C$ — tuning coefficient
$D$ — tuning coefficient
$a$ — coefficient
$b$ — coefficient
$c$ — coefficient
$d$ — coefficient
$P$ — pressure, kPa
$V$ — volume, cubic meter
$T$ — absolute temperature, K
$Z$ — compressibility factor
$N$ — number of kilomoles of the gas
$R$ — gas constant
$P_r$ — reduced pressure
$T_r$ — reduced temperature
$P_c$ — critical pressure, kPa
$T_c$ — critical temperature, K
$y_i$ — mole fraction of component $i$
$K$ — parameter
$P_{pc}$ — pseudo-critical pressure, kPa
$T_{pc}$ — pseudo-critical temperature, K
$\gamma_g$ — the specific gravity of gas
$\varepsilon$ — critical temperature correction, K

**References**