**DRANCHUK AND ABOU-KASSEM EQUATION OF STATE FOR CALCULATING GAS *Z*
FACTOR USING NEWTON'S AND THE SECANT NUMERICAL METHODS**

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0. Abstract.
Hydrocarbon reservoir calculations demands high accuracy and consequently hard work. There are two ways to obtain these results: numerical and graphical methods. Numerical methods cover several correlations and usually they have become trustworthy in the field. There are also several software provided by the oil industry, although they are usually expensive. On the other hand, graphical methods use diagrams in which accuracy depends upon designer's point of view.

The purpose of this project is to develop a practical tool for calculating one of the most common and important factors in Hydrocarbon Reservoir Engineering: the gas deviation factor, z. It will be necessary to use Newton's and the Secant Numerical Methods, and also it will include the development of a program in C++ or VBA. Some widely used software in the Petroleum Industry, such as Pipephase, NPTop use similar algorithms.

0.1. Importance of this project
The main objective of this project is to develop a simple and very practical tool for calculating the gas z factor based on numerical methods (Newton's and the Secant). There is software that can be easily found in websites, but this project not only computes the gas z factor, but also explains the theory supporting this equation.

0.2. Methodology
- Review theoretical background of gas z factor
- Review the Dranchuk and Abou-Kassem Equation of State for calculating Gas z Factor.
- Apply Newton's and the Secant methods to solve this equation.
- Develop algorithms and flowchart for any language programming.
- Software development (C++ or VBA)
- Test its results theoretically and compare them with those obtained by Standing and Katz Graphical Correlation.
- Make recommendations for its applicability.

0.3. Application.
Due to gas z factor is a very common input data for several correlations, it can be easily used on them, for example in the Cullendar and Smith Method (BHFP).

1. Theoretical background of gas *z* factor.
1.1 Ideal-Gas Law. An equation describing the relationship between the volume occupied by a gas and the pressure and temperature is called an equation of state (EOS). Combining Boyle's and Charles' laws, we obtain the EOS for an ideal gas:

$$p \cdot V = n \cdot R \cdot T \tag{Eq. 1.1}$$

Where p = pressure [psia]; V = volume [ft^3]; n = number of pound-moles of gas; R = universal gas coefficient = 10.732 $\left[\dfrac{psia \cdot ft^3}{^oR \cdot lb_m mol} \right]$; and T = absolute temperature, ^oR.

1.2 Real-gas behavior. The Real-gas law is simply the pressure/volume relation predicted by the ideal-gas law modified by a correction factor that accounts for the nonideal behavior of the gas. The real-gas law is:

$$p \cdot V = z \cdot n \cdot R \cdot T \tag{Eq. 1.2}$$

Where z = dimensionless quantity called the z factor. This corrects the simple Equation of State (EOS) for an ideal gas and allows us to describe the behavior of a real gas.

1.3 Principle of Corresponding States. Several gas properties have the same values for similar gases at identical values of reduced pressure and temperature. Reduced pressure and reduced temperature for pure compounds are defined as:

$$p_r = \frac{p}{p_c} \tag{Eq. 1.3}$$

$$T_r = \frac{T}{T_c} \tag{Eq. 1.4}$$

For gas mixtures , p_r and T_r are called Pseudoreduced pressure and pseudoreduced temperature and they are defined as:

$$p_{pr} = \frac{p}{p_{pc}} \tag{Eq. 1.5}$$

$$T_{pr} = \frac{T}{T_{pc}} \tag{Eq. 1.6}$$

Where p_c = critical pressure for a pure gas, [psia]; p_{pc} = pseudocritical pressure for a gas mixture, [psia]; T_c = critical temperature for a pure gas, [°R]; and T_{pc} = pseudocritical temperature for a gas mixture, [°R]. The critical point p_c, T_c for a pure substance is the pressure and temperature at which the properties of the liquid and vapor phases become identical. At pressures above p_c, liquid and gas cannot coexist, regardless of the temperature; at temperatures above T_c, the substance cannot be liquefied, regardless of the pressure. For pure substances, p_c and T_c are determined experimentally. For mixtures, p_{pc} and T_{pc} either are computed with some consistent set of mixing rules or are estimated from correlations.
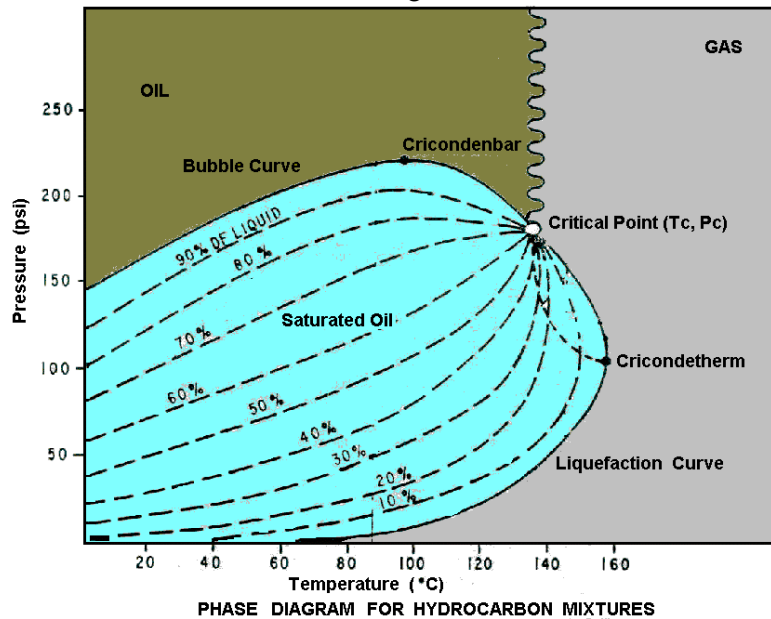
PHASE DIAGRAM FOR HYDROCARBON MIXTURES
Graph 1.1.

1.4. Sutton's Method for Calculating Pseudocritical Properties. When gas composition is unknown, the Sutton's method is a good device to estimate both Pseudocritical Temperature (T_c) and Pseudocritical Pressure (p_c). Sutton's method uses the following equations:

$$p_c = 756.8 - 131 \cdot \gamma_g - 3.6 \cdot \gamma_g^2 \tag{Eq. 1.7}$$

$$T_c = 169.2 + 349.5 \cdot \gamma_g - 74 \cdot \gamma_g^2 \tag{Eq. 1.8}$$

Where γ_g is the Specific Gravity of gas which is defined as the ratio of the densities of the gas and dry air when both are measured at the same pressure and temperature.

1.5 Standing and Katz Graphical Correlation. It is a function of the pseudoreduced pressure, p_r, and pseudoreduced temperature, T_r. The algorithm for this procedure is simple: after calculating p_r, and T_r, these values are entered in respective axis and in the intersection, it is obtained the z factor. This apparently easy procedure becomes tedious when repeating over and over again in correlations which need to calculate z factor.
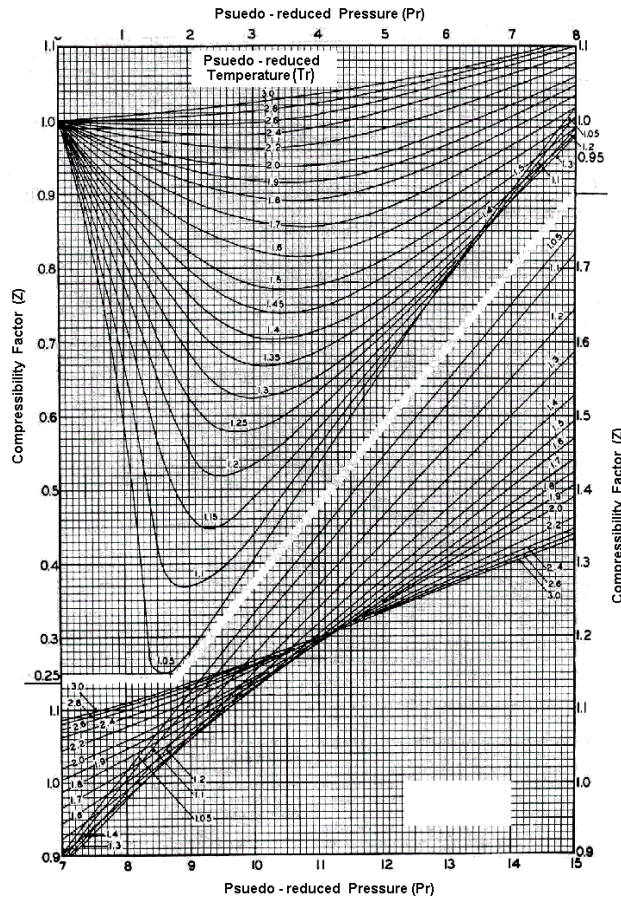
2. The Dranchuk and Abou-Kassem Equation of State for calculating Gas z Factor.
This is based in the following equations:

$$z = 1 + c_1 \cdot \rho_r + c_2 \cdot \rho_r^2 - c_3 \cdot \rho_r^5 + c_4 \tag{Eq. 2.1}$$

Where

$$\rho_r = \frac{0.27 \cdot p_r}{z \cdot T_r} \tag{Eq. 2.2}$$

$$c_1 = A_1 + \frac{A_2}{T_r} + \frac{A_3}{T_r^3} + \frac{A_4}{T_r^4} + \frac{A_5}{T_r^5} \tag{Eq. 2.3}$$

$$c_2 = A_6 + \frac{A_7}{T_r} + \frac{A_8}{T_r^2} \qquad \text{(Eq. 2.4)}$$

$$c_3 = A_9 \cdot \left(\frac{A_7}{T_r} + \frac{A_8}{T_r^2} \right), \text{ and} \qquad \text{(Eq. 2.5)}$$

$$c_4 = A_{10} \cdot \left(1 + A_{11} \cdot \rho_r^2 \right) \cdot \left(\frac{\rho_r^2}{T_r^3} \right) \cdot \exp\left(- A_{11} \cdot \rho_r^2 \right) \qquad \text{(Eq. 2.6)}$$

The constants A_1 through A_{11} are as follows:

$A_1=$ 0.32650
$A_2=$ -1.07000
$A_3=$ -0.53390
$A_4=$ 0.01569
$A_5=$ -0.05165
$A_6=$ 0.54750
$A_7=$ -0.73610
$A_8=$ 0.18440
$A_9=$ 0.10560
$A_{10}=$ 0.61340
$A_{11}=$ 0.72100

Dranchuk and Abou-Kassem fitted the EOS to 1,500 data points with an average absolute error of 0.486% when the z factor is a function of T_r and ρ_r. The z factor based on EOS is accurate within engineering accuracy over the following ranges: $0.2 \le p_r < 30$, $1.0 < T_r \le 3.0$

The Dranchuk and Abou-Kassem EOS must be solved iteratively because the z factor appears on both sides of the equation. The solution to this problem can be obtained by use of a root solving technique, such as Newton's method, or the secant method. The root solving procedure requires that we rearrange (Eq. 2.1) to the form.

$$f(z) = 0 \qquad \text{(Eq. 2.7)}$$

Rearranging (Eq. 2.1) gives

$$f(z) = z - \left(1 + c_1 \cdot \rho_r + c_2 \cdot \rho_r^2 - c_3 \cdot \rho_r^5 + c_4 \right) \qquad \text{(Eq. 2.8)}$$

Newton's and the secant methods require the first derivative of (Eq. 2.8) with respect to z at constant Pseudoreduced temperature, $\left[\dfrac{\partial f(z)}{\partial z} \right]_{T_r}$ Newton's method assumes that the derivative is evaluated analytically by explicit differentiation of the function $f(z)$. The procedure to derivate (Eq. 2.8) with respect to z is:

Doing from (Eq 2.2): $k_1 = \dfrac{0.27 \cdot p_r}{T_r}$, then: $\rho_r = \dfrac{k_1}{z}$, and

$$\partial \rho_r = -\frac{k_1}{z^2} \partial z \implies \partial \rho_r = -\frac{\rho_r}{z} \partial z \qquad \text{(Eq. 2.9)}$$

$$\left[\frac{\partial f(z)}{\partial z} \right]_{T_r} = 1 - c_1 \partial \rho_r - 2 c_2 \rho_r \partial \rho_r + 5 c_3 \rho_r^4 \partial \rho_r - c_4' \qquad \text{(Eq. 2.10)}$$

Rearranging (Eq. 2.6): $c_4 = \left(\dfrac{A_{10}}{T_r^3} \rho_r^2 + \dfrac{A_{10} A_{11}}{T_r^3} \cdot \rho_r^4 \right) \cdot \exp\left(-A_{11} \cdot \rho_r^2 \right)$ (Eq. 2.11)

Doing: $k_2 = \dfrac{A_{10}}{T_r^3}$, $k_3 = \dfrac{A_{10} A_{11}}{T_r^3}$, $k_4 = -A_{11}$ (Eq. 2.12)

(Eq. 2.12) in (Eq. 2.11)

$c_4 = \left(k_2 \rho_r^2 + k_3 \rho_r^4 \right) \cdot e^{k_4 \rho_r^2}$ (Eq. 2.13)

Using the rule: $(uv)' = u'v + uv'$ (Eq. 2.14)

And doing: $u = k_2 \rho_r^2 + k_3 \rho_r^4$, and $v = e^{k_4 \rho_r^2}$ (Eq. 2.15)

$u' = 2 k_2 \rho_r \, d\rho_r + 4 k_3 \rho_r^3 \, d\rho_r$, $v' = 2 k_4 \rho_r \, e^{k_4 \rho_r^2} \, d\rho_r$ (Eq. 2.16)

Using (Eq. 2.15) and (Eq. 2.16) in (Eq. 2.13)

$c_4' = \left(2 k_2 \rho_r \, d\rho_r + 4 k_3 \rho_r^3 \, d\rho_r \right) e^{k_4 \rho_r^2} + \left(k_2 \rho_r^2 + k_3 \rho_r^4 \right)\left(2 k_4 \rho_r \, e^{k_4 \rho_r^2} \, d\rho_r \right)$

$c_4' = 2 e^{k_4 \rho_r^2} \rho_r \, d\rho_r \left[\left(k_2 + 2 k_3 \rho_r^2 \right) + k_4 \left(k_2 \rho_r^2 + k_3 \rho_r^4 \right) \right]$ (Eq. 2.17)

Using (Eq. 2.9) and (Eq. 2.13) in (Eq. 2.17)

$c_4' = 2 e^{-A_{11} \rho_r^2} \rho_r \dfrac{A_{10}}{T_r^3} \left(-\dfrac{\rho_r}{z} \right) \left[\left(1 + 2 A_{11} \rho_r^2 \right) - A_{11} \left(\rho_r^2 + A_{11} \rho_r^4 \right) \right]$

$c_4' = -2 \dfrac{A_{10} \rho_r^2}{T_r^3 \, z} \left[1 + A_{11} \rho_r^2 - \left(A_{11} \rho_r^2 \right)^2 \right] \exp\left(-A_{11} \rho_r^2 \right)$ (Eq. 2.18)

Using (Eq. 2.9) and (Eq. 2.18) in (Eq. 2.10)

$\left[\dfrac{\partial f(z)}{\partial z} \right]_{T_r} = 1 + c_1 \dfrac{\rho_r}{z} + \dfrac{2 c_2 \rho_r^2}{z} - \dfrac{5 c_3 \rho_r^5}{z} + \dfrac{2 A_{10} \rho_r^2}{z \, T_r^3} \left[1 + A_{11} \rho_r^2 - \left(A_{11} \rho_r^2 \right)^2 \right] \exp\left(-A_{11} \rho_r^2 \right)$ (Eq. 2.19)

3. Newton's and the Secant methods.

3.1. Derivative. Geometrically, the derivative of a function can be interpreted as the slope of the graph of the function. Its calculation derives from the slope formula for a straight line, except that a limiting process must be used for curves. The formula for the slope of a straight line is $\tan(\theta) = \dfrac{y_{i+1} - y_i}{x_{i+1} - x_i}$ or $\tan(\theta) = \dfrac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$ (see Graph 1). For a curve, this ratio will depend upon where the points are chosen, reflecting the idea that a curve has a different slope at different points. To find the slope at a desired point, the choice of the second point needed to calculate the ratio represents a difficulty, because, in general, if the second point is far from the first, the ratio will represent an average slope along the portion of the curve cut off, rather than the slope at either point (see Graph 2). To get around this difficulty, a limiting process is used whereby the second 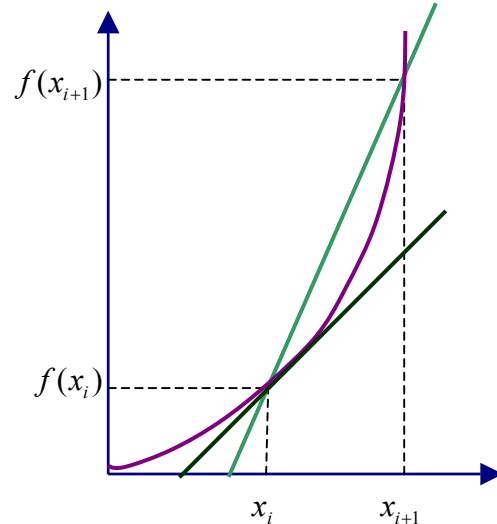point is not fixed but specified by $x_{i+1} - x_i$. When $x_{i+1} - x_i$ approaches 0, the limiting ratio will represent the actual slope at the given point.

To sum up, the derivative of $f(x_i)$, if this limit exists, is defined as:

$$\lim_{(x_{i+1} - x_i) \to 0} \dfrac{f(x_{i+1}) - f(x_i)}{(x_{i+1} - x_i)}$$ (Eq. 3.1)

$f(x_{i+1})$

$f(x_i)$

x_i x_{i+1}

Graph 3.1.

$f(x_{i+1})$

$f(x_i)$
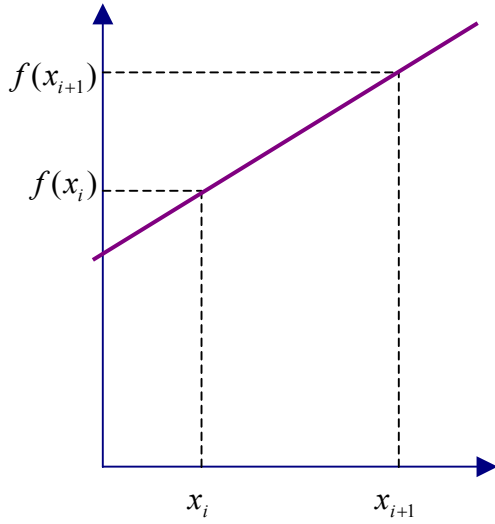
x_i x_{i+1}

Graph 3.2.

3.2. Approximation and Round–Off Errors. Truncation error are those resulting from using approximate estimates in place of the exact mathematical procedures. When analytically solutions are available, we have true error. When they are not available, we have apparent error. Round–Off error or computer error are those caused for computers because they can only represent quantities with a finite number of digits. There are other types of errors, including blunders, formulation or model error, and data uncertainty.

$$\varepsilon_t = \frac{true\ value - approximate\ value}{true\ value} \cdot 100\%$$ (Eq. 3.2)

$$\varepsilon_a = \frac{current\ approximation - previous\ approximation}{current\ approximation} \cdot 100\%$$ (Eq. 3.3)

As the apparent or true error becomes smaller, the closer the solution is to the true value. We use absolute value for the error. Due to iterative character of error estimation, a limit can be reached where in a tolerance can be specified ε_s
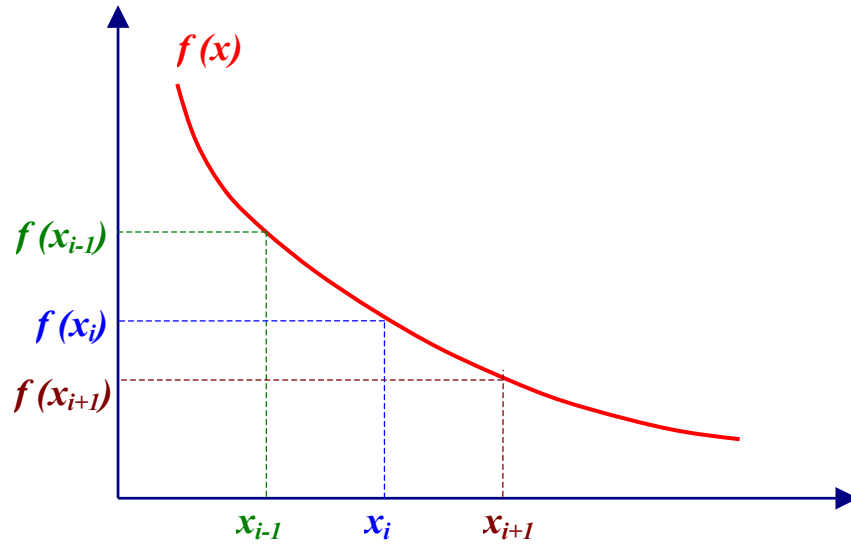
$$|\varepsilon_a| < \varepsilon_s$$ (Eq. 3.4)

ε_s is linked with the number of significant figures as follows:

$$\varepsilon_s = (0.5 \cdot 10^{2-n})\%$$ (Eq. 3.5)

Where, n is the number of significant figures (those can be used with confidence)

3.3. Taylor Series Expansion. Let us consider the following Graph:

Graph 3.3.

The Taylor's theorem states that any smooth function can be approximated by a polynomial. i.e. if the function f and its first $n+1$ derivatives are <u>continuous</u> on an interval containing x_i and x_{i+1}, then the value of the function at x_{i+1} is given by:

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)(x_{i+1} - x_i)^2}{2!} + \frac{f'''(x_i)(x_{i+1} - x_i)^3}{3!} + ... + \frac{f^n(x_i)(x_{i+1} - x_i)^n}{n!} + R_n$$

(Eq. 3.6)

Where R_n is defined as remainder. If R_n is neglected, then (Eq. 3.6) becomes the Taylor Polynomial Approximation to $f(x_{i+1})$. Taylor series is said to provide means to predict the value of function at one point in terms of the function value and its derivatives at another point:

0th – order Taylor: $f(x_{i+1}) = f(x_i)$

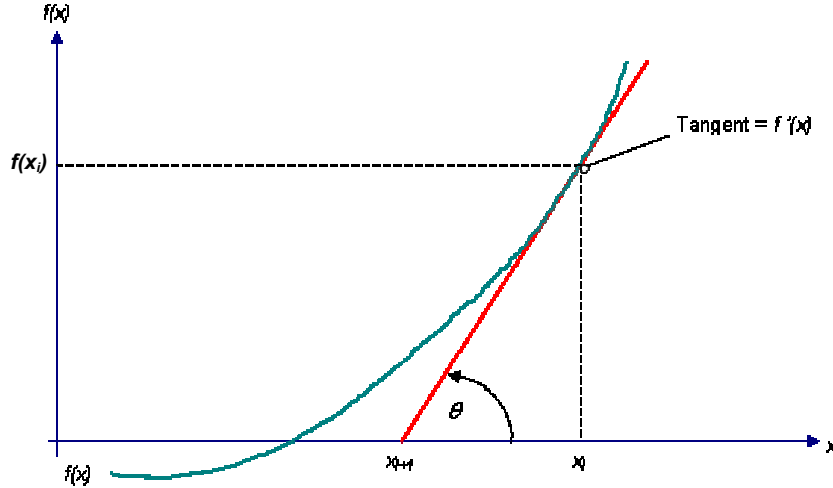1st – order Taylor: $f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i)$

2nd – order Taylor: $f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)(x_{i+1} - x_i)^2}{2!}$

3rd – order Taylor: $f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)(x_{i+1} - x_i)^2}{2!} + \frac{f'''(x_i)(x_{i+1} - x_i)^3}{3!}$

The term prediction can be used for both to predict the future or to predict the past. (Eq. 3.6) is used to predict the future and it is classified as Forward Difference Approximation. On the other hand, to predict the past, (Eq. 3.6) can be modified to give the Backward Difference Approximation.

3.4. The Newton-Raphson Method.

Graph 3.4.

a) Geometrically: $\tan(\theta) = f'(x_i) \Rightarrow f'(x_i) = \dfrac{f(x_i)}{(x_i - x_{i+1})}$

$\Rightarrow x_{i+1} = x_i - \dfrac{f(x_i)}{f'(x)}$

b) Using 1st – order Forward Difference Approximation: $f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) = 0$

$\Rightarrow x_{i+1} = x_i - \dfrac{f(x_i)}{f'(x_i)}$ \hfill (Eq. 3.7)

3.5. The Secant Method. This method is an extension of Newton – Raphson for cases where $f'(x)$ can not be analytically obtained.

Using 1st – order Backward Difference Approximation:

$f(x_{i-1}) = f(x_i) - f'(x_i)(x_i - x_{i-1}) = 0 \Rightarrow f(x_{i-1}) = f(x_i) + f'(x_i)(x_{i-1} - x_i) = 0$

$\Rightarrow f'(x_i) = \dfrac{f(x_{i-1}) - f(x_i)}{(x_{i-1} - x_i)}$ \hfill (Eq. 3.8)

(Eq. 3.8) in (Eq. 3.7):

$x_{i+1} = x_i - \dfrac{f(x_i)(x_{i-1} - x_i)}{f(x_{i-1}) - f(x_i)}$ \hfill (Eq. 3.9)

Notice that the approach requires two initial estimates of x.

4. General Algorithms
4.1. Algorithm for the Newton-Raphson Method.

$z_{i+1} = z_i - \dfrac{f(z_i)}{f'(z_i)}$ \hfill (Eq. 4.1)

$f(z_i) = z_i - \left(1 + c_1 \cdot \rho_r + c_2 \cdot \rho_r^2 - c_3 \cdot \rho_r^5 + c_4\right)$ \hfill (Eq. 4.2)

$f'(z_i) = 1 + c_1 \dfrac{\rho_r}{z_i} + \dfrac{2 c_2 \rho_r^2}{z_i} - \dfrac{5 c_3 \rho_r^5}{z_i} + \dfrac{2 A_{10} \rho_r^2}{z_i T_r^3}\left[1 + A_{11} \rho_r^2 - \left(A_{11} \rho_r^2\right)^2\right]\exp\left(- A_{11} \rho_r^2\right)$ \hfill (Eq. 4.3)

$$\rho_r = \frac{0.27 \cdot p_r}{z_i \cdot T_r}$$ (Eq. 4.4)

$$c_1 = A_1 + \frac{A_2}{T_r} + \frac{A_3}{T_r^3} + \frac{A_4}{T_r^4} + \frac{A_5}{T_r^5}$$ (Eq. 4.5)

$$c_2 = A_6 + \frac{A_7}{T_r} + \frac{A_8}{T_r^2}$$ (Eq. 4.6)

$$c_3 = A_9 \cdot \left(\frac{A_7}{T_r} + \frac{A_8}{T_r^2} \right)$$ (Eq. 4.7)

$$c_4 = A_{10} \cdot \left(1 + A_{11} \cdot \rho_r^2 \right) \cdot \left(\frac{\rho_r^2}{T_r^3} \right) \cdot \exp\left(- A_{11} \cdot \rho_r^2 \right)$$ (Eq. 4.8)

The constants A_1 through A_{11} are as follows:
A1=   0.32650
A2=   -1.07000
A3=   -0.53390
A4=   0.01569
A5=   -0.05165
A6=   0.54750
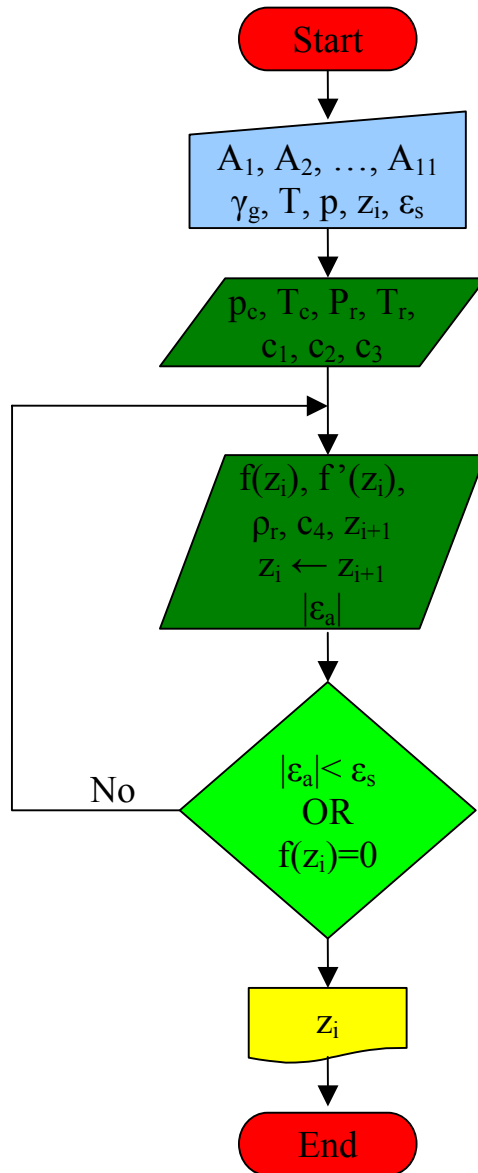A7=   -0.73610
A8=   0.18440
A9=   0.10560
A10=   0.61340
A11=   0.72100

4.2. Algorithm for the Secant Method.

$$z_{i+1} = z_i - \frac{f(z_i)(z_{i-1} - z_i)}{f(z_{i-1}) - f(z_i)}$$ (Eq. 4.9)

All other equations given in the algorithm for the Newton–Raphson method are applicable in this algorithm with exemption of (Eq. 4.1) and (Eq. 4.3)

4.3. Flow Charts.

Start

$A_1, A_2, \ldots, A_{11}$
$\gamma_g, T, p, z_i, \varepsilon_s$

$p_c, T_c, P_r, T_r,$
c_1, c_2, c_3

$f(z_i), f'(z_i),$
ρ_r, c_4, z_{i+1}
$z_i \leftarrow z_{i+1}$
$|\varepsilon_a|$

$|\varepsilon_a| < \varepsilon_s$
OR
$f(z_i)=0$

No

z_i

End

Graph 4.1

5. Conclusions

- After 100 tests, this equation fitted well with Standing and Katz graphical correlation, so its results can be used trusty as a good alternative.
- There are small differences (beyond significant figures) between Newton's Method and Secant. This can be explained if we consider these two methods are approximations.
- If we compare time to compute gas z factor using Standing and Katz graphical correlation and Dranchuk and Abou-Kassem Equation, there is a considerable saving. It takes about one minute as average, meanwhile Dranchuk and Abou-Kassem takes just few seconds.

6. References.

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