CM 3450
Assignment 1
Due: Sept. 8, 2008

Name: ____

1. **Word Equation Editor**. Use the key-stroke method to re-enter the enclosed document on root finding of cubic polynomials using Word 2007 and include equation numbers on all the equations.

2. **Data Tables.** Use the data table to obtain the compressibility factor of methane for $P_r = 0.1, 0.2, \ldots, 10$ at $T_r = 1, 1.2, 1.5, 2, 3$.

Obtaining the Roots of a Cubic Equations

Given a cubic equation,

$$z^3 + A \cdot z^2 + B \cdot z + C = 0$$

Let

$$z = x - \frac{A}{3}$$

then

$$x^3 + \left(\frac{-1}{3} \cdot A^2 + B\right) \cdot x + \frac{2}{27} \cdot A^3 + C - \frac{1}{3} \cdot B \cdot A = 0$$

or

$$x^3 + p \cdot x = q$$

where,

$$p = \left(\frac{-1}{3} \cdot A^2 + B\right)$$

$$q = -\left(\frac{2}{27} \cdot A^3 + C - \frac{1}{3} \cdot B \cdot A\right)$$

Further, let

$$x = y - \frac{p}{3y}$$

then we obtain a 6th order polynomial equation in y given by

$$y^6 - q \cdot y^3 - \frac{1}{27} \cdot p^3 = 0$$

whose roots are:

$$y = \left[\frac{q}{2} + \sqrt{\left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3}\right]^{\frac{1}{3}}$$

Now let the discriminant Δ be the term inside the square root above, i.e.

$$\Delta = \left(\frac{q}{2}\right)^2 + \left(\frac{P}{3}\right)^3$$

then we will have two cases that will depend on whether the discriminant is positive or negative.

Case 1: $\Delta > 0$ Then we will have one real root and a complex conjugate pair

The first root is given by

$$z_1 = sign(h)\cdot\left(|h|\right)^{\frac{1}{3}} - \frac{A}{3}$$

where,

$$h = \frac{q}{2} + \sqrt{\Delta}$$

The other roots can then be obtained by using the values of the first root:

$$z_2 = \frac{-\left(A + z_1\right) + \sqrt{\left(A + z_1\right)^2 - 4\cdot\left[B + z_1\cdot\left(A + z_1\right)\right]}}{2}$$

$$z_3 = \frac{-\left(A + z_1\right) - \sqrt{\left(A + z_1\right)^2 - 4\cdot\left[B + z_1\cdot\left(A + z_1\right)\right]}}{2}$$

Case 2: $\Delta < 0$ There will be three real roots.

The first root will be obained as follows (whose proof is given below):

$$z_1 = \left[2\cdot\left(\sqrt{\frac{-p}{3}}\right)\right]\cdot\cos\left(\frac{atan\left(\frac{\sqrt{-\Delta}}{\frac{q}{2}}\right)}{3}\right) - \frac{A}{3}$$

And the two remaining roots can be determined by the following equations:

$$z_2 = \frac{-\left(A + z_1\right) + \sqrt{\left(A + z_1\right)^2 - 4\cdot\left[B + z_1\cdot\left(A + z_1\right)\right]}}{2}$$

$$z_3 = \frac{-\left(A + z_1\right) - \sqrt{\left(A + z_1\right)^2 - 4\cdot\left[B + z_1\cdot\left(A + z_1\right)\right]}}{2}$$

Proof for formula to obtain the first root:

Let $h = \frac{q}{2} + i\sqrt{-\left(\frac{q}{2}\right)^2 - \left(\frac{p}{3}\right)^3}$

whose magnitude and angle are given by

$$|h| = \sqrt{\left(\frac{-p}{3}\right)^3}$$

$$\theta = arg(h) = atan\left(\frac{\sqrt{-\Delta}}{\frac{q}{2}}\right)$$

allowing one to evaluate the cube root of the polar representation:

$$y = h^{\frac{1}{3}} = \sqrt{\frac{-p}{3}}\cdot e^{i\cdot\frac{\theta}{3}}$$

from which we obtain

$$x = \sqrt{\frac{-p}{3}}\cdot e^{i\cdot\frac{\theta}{3}} + \frac{\frac{-p}{3}}{\sqrt{\frac{-p}{3}}\cdot e^{i\cdot\frac{\theta}{3}}}$$

$$x = \sqrt{\frac{-p}{3}} \cdot \left(e^{i \cdot \theta} + e^{-i \cdot \theta}\right) = 2 \cdot \sqrt{\frac{-p}{3}} \cdot \cos\left(\frac{\theta}{3}\right)$$

or

$$z_1 = x - \frac{A}{3} = 2 \cdot \sqrt{\frac{-p}{3}} \cdot \cos\left(\frac{\theta}{3}\right) - \frac{A}{3}$$

Compressibility Factor from Redlick-Kwong Equations

(Dr. Tom Co 9/2/08)

Working Equations:

(based on Cutlip and Shacham, 2008, pp. 101-103)

Let P be pressure in atm, T be temperature in K and $\hat{V}$ be molar volume in $\frac{liters}{g-mol}$. The Redlich-Kwong equation is given by

$$P = \frac{RT}{\hat{V} - b} - \frac{a}{\hat{V}(\hat{V} + b)\sqrt{T}} \tag{1}$$

where

$$a = 0.42747\left(\frac{R^2 T_c^{\frac{5}{2}}}{P_c}\right) \tag{2}$$

$$b = 0.08664\left(\frac{RT_c}{P_c}\right) \tag{3}$$

Suppose we want to obtain compressibility factor

$$z = \frac{P\hat{V}}{RT} \tag{4}$$

as a function reduced pressure $P_r = P/P_c$, at various cases of reduced temperature $T_r = T/T_c$.

First, solve for $\hat{V}$ in (4),

$$\hat{V} = \frac{zRT}{P} \tag{5}$$

then substitute (5) in (1) to obtain a cubic equation in z given by

$$z^3 - z^2 - qz - r \tag{6}$$

where,

$$r = AB \tag{7}$$

$$q = B^2 + B - A \tag{8}$$

$$A = 0.42747\left(\frac{P_r}{T_r^{\frac{5}{2}}}\right) \tag{9}$$

$$B = 0.08664\left(\frac{P_r}{T_r}\right) \quad (10)$$

If we wish to obtain the compressibility factor of the vapor phase, we need the maximum real-valued root of the cubic equation.

The mcroot Function:

The following code is a function to obtain the maximum real root of a cubic equation:

```
Function mcroot(a3, a2, a1, a0)
'
'   Computes the maximum real root of the cubic equation
'                   a3 x^3 + a2 x^2 + a1 x + a0 = 0
'
    Dim A, B, C, D, z
    A = a2 / a3
    B = a1 / a3
    C = a0 / a3
    p = (-A ^ 2 / 3 + B) / 3
    q = (9 * A * B - 2 * A ^ 3 - 27 * C) / 54
    Disc = q ^ 2 + p ^ 3
    If Disc > 0 Then
        h = q + Disc ^ (1 / 2)
        y = (Abs(h)) ^ (1 / 3)
        If h < 0 Then y = -y
        z = y - p / y - A / 3
    Else
        theta = Atn((-Disc) ^ (1 / 2) / q)
        c1 = Cos(theta / 3)
        If q < 0 Then
            s1 = sin(theta / 3)
            c1 = (c1 - s1 * 3 ^ (1 / 2)) / 2
        End If
        z1 = 2 * (-p) ^ (1 / 2) * c1 - A / 3
        m = A + z1
        r = (m ^ 2 - 4 * (B + m * z1)) ^ (1 / 2)
        z2 = (-m + r) / 2
        z3 = (-m - r) / 2
        z = z1
        If z2 > z Then z = z2
        If z3 > z Then z = z3
    End If
    mcroot = z
End Function
```

Figure 1. **mcroot** Code.

To include the function in an Excel worksheet:

1. Open the worksheet.
2. Press **[Alt-F11]** to open the VBA editor.
3. Click on the module (if it does not exist click **[Insert]→[Module]** to create).
4. Copy (or cut-and-paste) the function code above into the code window.
5. Press **[Alt-F11]** once more to go back to Excel worksheet.
6. Test the function.

Example: Compressibility of Steam for $P_r = 0.1, 0.2, \ldots, 10$ at $T_r = 1, 1.2, 1.5, 2, 3$.

	A	B	C	D	E	F	G	H
1	Component		Steam					
2		R	0.08206					
3		Tc	647					
4		Pc	218					
5		Pr	1.2					
6		Tr	1					
7		A	0.512964					
8		B	0.103968					
9		q	-0.39819					
10		r	0.053332					
11		z	0.25788					
12								
13				Tr=1	Tr=1.2	Tr=1.5	Tr=2	Tr=3
14			0.25788	1	1.2	1.5	2	3
15			0.1	0.965162	0.979972	0.990293	0.996817	1.000162
16			0.2	0.928637	0.959637	0.980652	0.993718	1.000356
110			9.6	1.206428	1.137806	1.107138	1.118883	1.136462
111			9.7	1.216871	1.146476	1.113608	1.122948	1.138788
112			9.8	1.227301	1.155138	1.120084	1.127031	1.141125
113			9.9	1.237718	1.163792	1.126568	1.131134	1.143473
114			10	1.248122	1.172438	1.133057	1.135255	1.145832

=mcroot(1,-1,-C9,-C10)

Figure 2. Data table for compressibility factors.

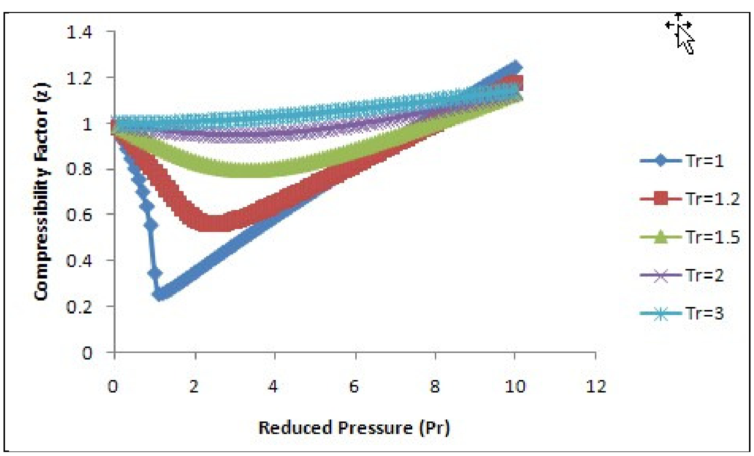

Figure 3. Compressibility chart.