CM3450
Fall 2008
Drill 7

1. Symbolic Manipulation.

Given the Peng-Robinson equation:

$$P = \frac{R_g T}{V - b} - \frac{a\alpha}{V^2 + 2bV - b^2} \tag{1}$$

$$z = \frac{PV}{R_g T} \tag{2}$$

where

$$a = 0.45724 \frac{T_c^2}{P_c} \qquad b = 0.07780 \frac{R_g T_c}{P_c}$$

$$\alpha = \left(1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)\left(1 - \sqrt{T_r}\right)\right)^2$$

Show that from both (1) and (2),

$$z^3 - (1 - B)z^2 + (A - 3B^2 - 2B)z - (AB - B^2 - B^3) = 0 \tag{3}$$

where,

$$A = \frac{\alpha a P}{R_g^2 T^2} \qquad B = \frac{bP}{R_g T}$$

Procedure using MathCad:

a) Type the equation for z (remember to use **[crtl =]**). Position cursor next to V then **[Symbolic]→[Variable]→[Solve]**.
b) Type the following equation

$$\left(P - \left[\frac{RT}{V - b} - \frac{a\alpha}{V^2 + 2bV - b^2}\right]\right)(V - b)(V^2 + 2bV - b^2)$$

c) Select the complete equation above then **[Symbolic]→[Expand]**.
d) Position cursor next to V then **[Symbolic]→[Collect]**.
e) Select and copy the earlier solution found for V in terms of z, then position the cursor next to V and then **[Symbolic]→[Variable]→[Substitute].**
f) Divide the whole result by inserting the following into the divisor: $\frac{R_g^3 T^3}{P^2}$
g) Position the cursor next to z, then **[Symbolic]→[Polynomial coefficients]**.
h) Insert terms as shown in Figure 1.

$$\begin{bmatrix} \left(\frac{-P^2}{R_g^3 \cdot T^3} \cdot a \cdot \alpha \cdot b + \frac{P^2}{R_g^2 \cdot T^2} \cdot b^2 + \frac{P^3}{R_g^3 \cdot T^3} \cdot b^3\right) + \left(A \cdot B - B^3 - B^2\right) \\ \left(\frac{-2}{R_g \cdot T} \cdot P \cdot b - 3 \cdot \frac{P^2}{R_g^2 \cdot T^2} \cdot b^2 + \frac{P}{R_g^2 \cdot T^2} \cdot a \cdot \alpha\right) - \left(A - 3B^2 - 2B\right) \\ \left[(-1) + \frac{1}{R_g \cdot T} \cdot P \cdot b\right] + (1 - B) \\ 1 - 1 \end{bmatrix}$$

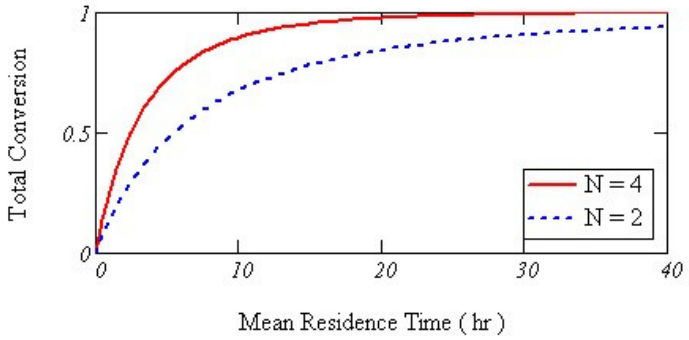
Figure 1

i) Key-in **[crtl shift period]**, and in the placeholder, type the following:

$$substitute, B = \frac{b \cdot P}{R_g \cdot T}, A = \frac{a \cdot \alpha \cdot P}{R_g^2 \cdot T^2}$$

The result should be all zeros.

2. Plotting. Exercise #7 (page 22).
   Procedure:
   a) Solve for X and write as function of k, τ and N.
   b) Make a series for $\tau := 0,0.5..40$
   c) Insert x-y graph (or hit "@" key). In the x-axis, enter τ, while in the y-axis, enter $X(0.075, \tau, 4)$.
   d) Next to the first y-axis function, enter a comma, then enter $X(0.075, \tau, 2)$.
   e) Try modifying the plot to : include legend, hide arguments, include labels:



3. Importing and exporting data.
   a) Try importing the data you used during drill 5: **antoine_data1.txt** .
   b) Next, extract the first column as variable T and the second column as variable P.
   c) Now build a new matrix by augmenting the two data with P in the first column and T in the second.
   d) Next try exporting the new matrix as Test.txt.