PETR 6328: Problem Set #3

Instructor: Dr. B. Dindoruk, University of Houston

Due Date: October 27, 2015

Problem Statement:

Write a program/implementation that calculates the compositions and molar volumes (densities) of two phases in equilibrium for the quaternary system given below (you need to write a two-phase flasher with Soave-Redlich-Kwong and Peng-Robinson EOS capabilities – see Problem Set # 2).

- Document your work and outline the process. Presentation should be neat and professional (tables, plots etc, as needed).
- Use the fugacity expression from Problem Set #2 (also given below)
- Include **source code/listing** and executable(s) (This is a must) and relevant details how to run the program/implementation + again how you have completed the work
- Please submit all your work electronically using blackboard (pls. pack all the files together to make it easier to download).

Flash Conditions:

Temperature: 180 °F
Pressure: 2000 psia

Mixture Composition :

CO2 : 0.65 (mole fraction)
CH4 : 0.20 (mole fraction)
n-C4 : 0.05 (mole fraction)
n-C10 : 0.10 (mole fraction)

INPUT DATA

Binary Interaction Parameters (PREOS):

kij	CO2	CH4	n-C4	n-C10
CO2	0	0.1200	0.1200	0.1141
CH4	0.1200	0	0.0000	0.0422
n-C4	0.1200	0.0000	0	0.0078
n-C10	0.1141	0.0422	0.0078	0

Binary Interaction Parameters (SRKEOS):

kij	CO2	CH4	n-C4	n-C10
CO2	0	0.1200	0.1200	0.1304
CH4	0.1200	0	0.0000	0.0411
n-C4	0.1200	0.0000	0	0.0067
n-C10	0.1304	0.0411	0.0067	0

Component	MW	Tc (F)	Pc (psi)	Acentric Factor (ω)	Cpen (ft3/lb-mol) FOR PREOS (Optional)	Cpen (ft3/lb-mol) FOR SRKEOS (Optional)
CO2	44.010	87.890	1069.87	0.2250	-2.63E-02	4.85E-02
CH4	16.043	-116.590	667.20	0.0080	-8.33E-02	1.01E-02
n-C4	58.124	305.690	551.10	0.1930	-0.10	0.13
n-C10	142.285	652.010	305.68	0.4900	0.26	0.68

Fugacity expression for the generalized cubic $P = \frac{RT}{V-b} - \frac{a\alpha}{V^2 + ubV + wb^2}$ (as defined in Homework #2) is :

$$\ln \hat{\phi}_i = \ln \frac{\hat{f}_i}{y_i P} = \frac{B_i}{B}(Z-1) - \ln(Z-B) + \frac{A}{B\sqrt{u^2-4w}}\left[\frac{B_i}{B} - \delta_i\right] \ln\left(\frac{2Z + B(u+\sqrt{u^2-4w})}{2Z + B(u-\sqrt{u^2-4w})}\right) \quad \mathrm{i} = 1,2,...,\mathrm{n_c}$$

Where

$$A = \frac{(a\alpha)P}{R^2T^2}, \qquad B = \frac{bP}{RT}$$

and

$$\delta_i = \frac{2}{(a\alpha)} \sum_{j=1}^{n_c} y_j (a\alpha)_{ij} \quad \mathrm{i} = 1,2,...,\mathrm{n_c}$$

With the following mixing rules

$$b = \sum_{i=1}^{n_c} y_i b_i \qquad \text{and} \qquad (a\alpha) = \sum_{i=1}^{n_c}\sum_{i=1}^{n_c} y_i y_j (a\alpha)_{ij}$$

$$(a\alpha)_{ij} = (1-k_{ij})\sqrt{(a\alpha)_i (a\alpha)_j}$$

The general form of the cubic EOS in terms of Z – factor $\left(Z = \frac{PV}{RT}\right)$

$$Z^3 - (1 + B - uB)Z^2 + (A + wB^2 - uB - uB^2)Z - AB - wB^2 - wB^3 = 0$$

For example, for Peng-Robinson EOS (u=2, and w= -1), the generalized fugacity coefficient equation for the cubic EOS shown above can be expressed as:

$$\ln \hat{\phi}_i = \ln \frac{\hat{f}_i}{y_i P} = \frac{B_i}{B}(Z-1) - \ln(Z-B) + \frac{A}{2\sqrt{2}B}\left[\frac{B_i}{B} - \frac{2}{(a\alpha)} \sum_{j=1}^{n_c} y_j (a\alpha)_{ij}\right] \ln\left(\frac{Z + B(1+\sqrt{2})}{Z + B(1-\sqrt{2})}\right) \quad \mathrm{i} = 1,2,...,\mathrm{n_c}$$

where

$$A = \frac{(a\alpha)P}{R^2T^2}, \qquad B = \frac{bP}{RT} \quad , \qquad \hat{\phi}_i = \frac{\hat{f}_i}{y_i P}$$ (these definitions are the same as in the case of the general form - of the EOS)

For PREOS, Z is the root of the following cubic equation:

$$Z^3 - (1-B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0$$

ANSWERS:

Using SRK EOS with no volume translation:

V= 0.6488523 mol, Z_v = 0.7002532, Molar Volume of Vapor (V_v) = 2.4035881 ft3/lb-mole
L= 0.3511477 mol, Z_l = 0.5709956, Molar Volume of Liquid (V_l) = 1.9599173 ft3/lb-mole

Component	**Zi (Feed mol frac)**	**yi (vap mol frac)**	**xi (liq mol frac)**	**K_i = yi/xi**	**Partial Fugacity, $\hat{f}_i$ (psi)**
CO2	0.65	0.716034	0.527981	1.35617E+00	9.85190E+02
CH4	0.20	0.237363	0.130961	1.81247E+00	5.07354E+02
n-C4	0.05	0.034123	0.079337	4.30101E-01	1.88295E+01
n-C10	0.10	0.012480	0.261720	4.76834E-02	7.10339E-01

Using PR78 EOS with no volume translation:

V= 0.6550856 mol, Z_v = 0.658278, Molar Volume of Vapor (V_v) = 2.25951051 ft3/lb-mole
L= 0.3449143 mol, Z_l = 0.511646, Molar Volume of Liquid (V_l) = 1.75620281 ft3/lb-mole

Component	**Zi (Feed mol frac)**	**yi (vap mol frac)**	**xi (liq mol frac)**	**K_i = yi/xi**	**Partial Fugacity, $\hat{f}_i$ (psi)**
CO2	0.65	0.713949	0.528543	1.35079E+00	9.3606E+02
CH4	0.20	0.236146	0.131349	1.79785E+00	4.8389E+02
n-C4	0.05	0.035110	0.078280	4.48518E-01	1.7614E+01
n-C10	0.10	0.014795	0.261828	5.65055E-02	6.6118E-01