Sharif University of Technology
Department of Chemical and Petroleum Engineering

Assignment (2) Report

- Multiphase Flow Fluid Mechanics -

By Radman Hosseinzadeh
Student #98206364
April 16, 2020

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Ppc (MPa)	Tpc (K)	ω
1.84	720.17	0.647

Table 1: C7+ properties

1 Methodology

Firstly, it should be noted that for ease of application, all units of pressure and temperature are converted to MPa and Kelvin, respectively. So the flash pressure is equal to 6.89476 MPa and flash temperature is 327.594 Kelvin. The gas constant R is also equal to 8.314×10^{-3} $L.MPa/K/mole$.

Furthermore, vectorization is used in the code as opposed to looping, so for example, the parameter Z is a 1 by 7 row-vector connecting each respective component to its fraction in the mixture. Same goes for K, a, b, etc.

1.1 Pseudocritical Properties and Acentric Factor of C7+

After entering the data provided by the problem, the first step is to calculate pseudo-critical parameters of the C7+ section. For this purpose, some parameters have been identified, including: TB, Ppc, and Tpc, which are defined using Eq. B-12 to B-14 of [2] and by having the specific gravity and molecular weight of the C7+ mixture.

Furthermore, the acentric factor is obtained via Eq. 5.60 of [4] knowing the critical properties and boiling temperature of the C7+ section. These derived values are demonstrated in Table 1. Therefore, the acentric factors and critical properties of the whole mixture is known from the above-mentioned process and Table A.1. of [1]. Reduced pressures and temperatures are then calculated.

1.2 Step-by-Step Calculations

Now, in the first formal step of the flash calculation algorithm drawn in Figure 1, K is estimated based on Eq. 3.66 of the book.

$$K = (1/Pr) \times exp(5.37(1+\omega)(1-(1/Tr)))$$

Where the value for β, the fraction of gas phase (n^V), is calculated through solving the Rachford-Rice equation via Newton-Raphson numerical method given in Eq. 6.22-24 of [3]. There has been two 'if' statements embedded afterwards to evaluate the phase of the mixture; Eq. 5.7-8 of the book should be satisfied for the fluid to be in a two-phase state and the Rachford-Rice equation to yield a physically correct root for β. Subsequently, component fractions of each phase, x, and y, are calculated as

$$x = \frac{Z}{1+(K-1)\beta}$$

and

$$y = Kx$$

The third step begins with calculating m, a, and b parameters for each component of to obtain Z-factor of the gas phase based on Peng-Robinson EOS, and eventually get the fugacity coefficient for this phase. The gas phase Z-factor is obtained via the procedure discussed in Assignment (1), and is stored in the parameter Zg, however the a, and b parameters are different due to the fluid being a mixture. So, it is customary to calculate the mixture a, and b using Eq. 4.78 and 4.74, respectively.

$$b = \sum_i y_i b_i$$

and

$$a = \sum_j \sum_i y_i y_j (a_i.a_j)^{0.5} \times (1 - k_{ij})$$

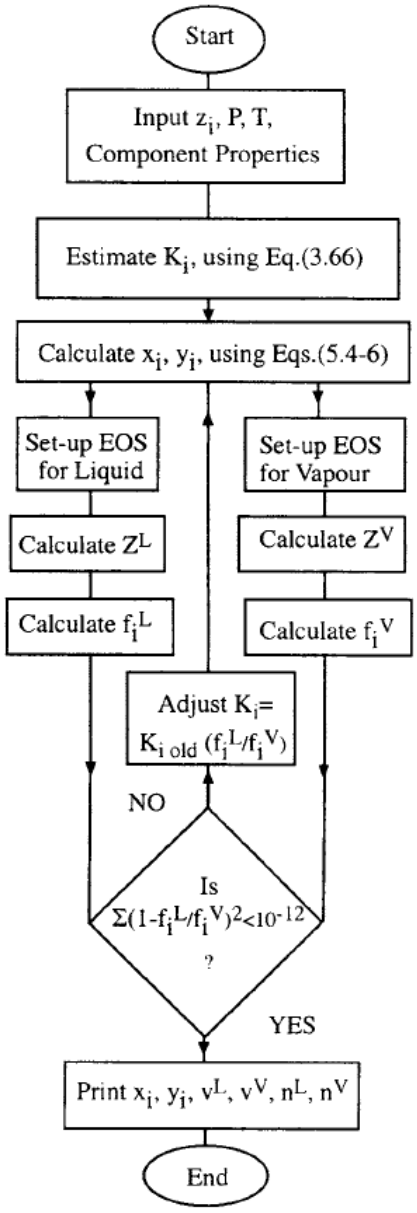

Figure 1: Flash calculation flow-chart [1]

Where k_{ij} is the Binary Interaction Parameter (or BIP as is mentioned in the code) is a 7 by 7 matrix allocating each couple of components a coefficient which is gathered based on Table A.4.3. of the source book. It should be noted that for the BIP for C7+ components are assumed to be equal to the BIP for nC10-nC14.

When Z-factor is obtained, the fugacity coefficient is derived via Eq. E5.2 of the reference paper. (line 122) A similar process is carried out using y instead of x in the formulation to calculate the Z-factor for the

	Gas Phase Composition (y_i)	Liquid Phase Composition (x_i)
C1	0.81	0.19
C2	0.11	0.086
C3	0.056	0.103
nC4	0.017	0.079
nC5	0.0051	0.052
nC6	0.0022	0.050
C7+	3.64×10^{-5}	0.44

Table 2: Gas and liquid phase composition after flash calculation.

liquid phase as well. Then the liquid fugacity is calculated via Eq. E5.2 using liquid phase Z-factor, liquid phase a and b, and x.

1.3 Iteration and Error Criteria

As the final step, the fugacities for each phase are calculated by

$$f_i^V = \phi_i^V y_i P_i$$

and

$$f_i^L = \phi_i^L x_i P_i$$

and according to the flow-chart presented in Figure 1 the criteria should be a sum of squared errors less than 10^{-12} and the error itself is defined as

$$\sum (1 - f_i^L / f_i^V)^2$$

So, based on the obtained fugacities, the above term is calculated and attempted to minimize by performing iteration on the vector K, adjusting it to

$$K = K \times (f_i^L / f_i^V)$$

and looping to re-calculate β, x, y, and so on until convergence occurs.

2 Results

The application generates a table of results including information about each component's fraction in liquid and gas phases and the molar amounts of each phase. The results are illustrated in Table 2. The code achieved this results after 8 iterations, altering K.

The molar amount of gas phase is derived to be $\beta = n^V = 0.306$ and the liquid phase molar amount, n^L, is equal to $1 - \beta = 0.694$. The generated values of molecular weight for the gas and liquid phase are 20.33 and 110.59 kg/kgmole, respectively.

References

[1] Ali Danesh. *PVT and phase behaviour of petroleum reservoir fluids*. Elsevier, 1998.

[2] W.D. McCain. *The Properties of Petroleum Fluids*. PennWell Books, 1990.

[3] Karen Schou Pedersen, Peter Lindskou Christensen, and Jawad Azeem Shaikh. *Phase behavior of petroleum reservoir fluids*. CRC press, 2014.

[4] Curtis H Whitson, Michael R Brulé, et al. *Phase behavior*, volume 20. Henry L. Doherty Memorial Fund of AIME, Society of Petroleum Engineers ..., 2000.