جامعة الملك سعود
King Saud University

كلية الهندسة
جامعة الملك سعود
King Saud University
College Of Engineering

Properties of Reservoir Fluids (PGE 362)

Quantitative Phase Behavior

BY
DR. MOHAMMED A. KHAMIS
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Ideal Solutions

Multi-component system:

Bubble point for two-components.

$$BPP = x_1 P_1^{\circ} + x_2 P_2^{\circ}$$

Raoult's Law can be expanded for multi-components system,

$$BPP = \sum x_i P_i^{\circ}$$

$$y_i = \frac{P_i}{P_T} = \frac{x_i P_i^{\circ}}{BBP}$$

Ideal Solutions

Multi-component system:

If:

n = total number of moles in the system

n_l = total number of moles in the liquid

n_v = total number of moles in the vapor

z_i = mole fraction of ith component in the overall system

x_i = mole fraction of ith component in the liquid

y_i = mole fraction of ith component in the vapor

Then:

$z_i n$ = moles of ith component in the system

$x_i n_l$ = moles of ith component in the liquid

$y_i n_v$ = moles of ith component in the vapor

Ideal Solutions

Multi-component system:

Material balance of the i[th] component:

$$z_i n = x_i n_l + y_i n_v$$

Applying Raoult's Law and Dalton's Law to of the i[th] component:

$$y_i = \frac{P_i}{P_T} = \frac{x_i P_i^\circ}{P_T}$$

Elimination of y_i and solving for x_i:

$$z_i n = x_i n_l + \frac{P_i^\circ}{P_T} x_i n_v$$

$$x_i = \frac{z_i n}{n_l + \frac{P_i^\circ}{P_T} n_v}$$

Ideal Solutions

Multi-component system:

Material balance of the i[th] component:

Since $\sum x_i = 1$:

$$\sum x_i = \sum \frac{z_i n}{n_l + \frac{P_i^\circ}{P_T} n_v} = 1$$

Elimination of x_i and solving for x_i:

$$\sum y_i = \sum \frac{z_i n}{n_v + \frac{P_T}{P_i^\circ} n_l} = 1$$

Ideal Solutions

Multi-component system:

These two equations are equivalent and either one can be used to calculate the compositions of a two-phase multicomponent system. These equations are most readily solved by trial and error. To simplify the calculation, one mole of starting material is taken as a basis. In this case $n = 1$ and $n_l + n_v = 1$. A reasonable value of n_l or n_v is chosen and the required summation at the temperature and pressure in question is carried out using equation 12 or 13. If the sum is equal to one then each term in the sum is equal to x_i or y_i, depending on which equation was employed. If the summation does not equal one a second value of n_l or n_v must be chosen and the computation repeated.

Ideal Solutions

Multi-component system:

EXAMPLE. A system consists of 25 mole per cent propane, 30 mole per cent pentane and 45 mole per cent heptane at 150° F. Assuming ideal solution behavior calculate the composition of the liquid and the vapor at 20 psia.

Let $n = 1$ and assume $n_l = 0.45$. Then $n_v = 0.55$ and the following calculations are carried out according to equation 12.

(1) Component	(2) z_i	(3) P_i^0	(4) $\frac{P_i^0}{P_T} = \frac{P_i^0}{20}$	(5) $x_i = \frac{z_i}{0.45 + (P_i^0/20)0.55}$
C_3H_8	0.25	345.0	17.25	0.025
C_5H_{12}	0.30	36.6	1.83	0.207
C_7H_{16}	0.45	5.0	0.25	0.766
				$\Sigma x_i = 0.998$

Ideal Solutions

Multi-component system:

Solution:

Since Σx_i is essentially equal to one the composition of the liquid is given in column 5. It is understood that if the sum had not been equal to one another value of n_l would be assumed. The composition of the vapor can be calculated using equation 13 and substituting $n = 1$, $n_l = 0.45$, and $n_v = 0.55$. However, it is simpler to apply equation 11 directly and, since x_i for each component is now known, the values of y_i may be computed. The composition of the vapor calculated in this manner is given below.

x_i	$y_i = \dfrac{x_i P_i^0}{P_T}$
0.025	$17.25 \times 0.025 = 0.431$
0.207	$1.83 \times 0.207 = 0.379$
0.766	$0.25 \times 0.766 = 0.191$