

## Properties of Reservoir Fluids (PGE 362)

# Quantitative Phase Behavior

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# Ideal Solutions

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## 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

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## Two components 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  $i^{\text{th}}$  component in the overall system

$x_i$  = mole fraction of  $i^{\text{th}}$  component in the liquid

$y_i$  = mole fraction of  $i^{\text{th}}$  component in the vapor

Then:

$z_i n$  = moles of  $i^{\text{th}}$  component in the system

$x_i n_l$  = moles of  $i^{\text{th}}$  component in the liquid

$y_i n_v$  = moles of  $i^{\text{th}}$  component in the vapor

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## Multi-components system:

Material balance of the  $i^{\text{th}}$  component:

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

Applying **Raoult's Law** and Dalton's Law to of the  $i^{\text{th}}$  component:

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

Elimination of  $y_i$  and solving for  $x_i$ :

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

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

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## Multi-component system:

Material balance of the  $i^{\text{th}}$  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

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## 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)	(2)	(3)	(4)	(5)
Component	$z_i$	$P_i^0$	$\frac{P_i^0}{P_T} = \frac{P_i^0}{20}$	$x_i = \frac{z_i}{0.45 + (P_i^0/20)0.55}$
$C_3H_8$	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  $\sum x_i$  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.

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