# Illustrative Example

# Recap

We derived the following equations:
Split fractions:

$$\xi_k = \frac{\alpha_{k/n}\xi_n}{1 + (\alpha_{k/n} - 1)\xi_n}$$

Simplified bubble-point equation: $\frac{P_k^0}{P} = \frac{\alpha_{k/n}}{\bar{\alpha}}$

Simplified dew-point equation: $\sum_{i=1}^{n} \frac{y_i}{\alpha_{i/n}} = \frac{P_n^0}{P}$

Vapor Fraction and Split Fraction:

$$\xi_n = \frac{1}{\frac{1}{K_n\phi} - \frac{1}{K_n} + 1}$$

How are these equations useful in solving the flash model?

In particular, how do we use these equations in the following scenarios?

| | |
|---|---|
| $T_V,\ P_V$ specified | Isothermal flash |
| $V/F = 0,\ P_L$ specified | Bubble point temperature |
| $V/F = 1,\ P_V$ specified | Dew point temperature |
| $T_L$ specified, $V/F = 0$ | Bubble point pressure |
| $T_V$ specified, $V/F = 1$ | Dew point pressure |
| $Q = 0,\ P_V$ specified | Adiabatic flash |
| $Q, P_V$ specified | Nonadiabatic flash |
| $V/F,\ P_V$ specified | Percent vaporization flash |

# Illustrative Example

Consider the mixture with components, flowrates, boiling points and Antoine coefficients given in the following table:

| Comp., $k$ | $f_k$ $(kmol/hr)$ | B. pt. $(K)$ | $A_k$ | $B_k$ | $C_k$ |
|---|---|---|---|---|---|
| Benzene, 1 | 30 | 353 | 15.9008 | 2778.51 | -52.34 |
| Toluene, 2 | 50 | 383 | 16.0137 | 3096.52 | -53.67 |
| O-xylene, 3 | 20 | 418 | 16.1156 | 3395.57 | -59.4 |

where the Antoine equation is given by:

$$ln(P_k^0) = A_k - \frac{B_k}{(C_k + T)}$$

where $P_k^0$ is in $mm\ Hg$ and $T$ is in $K$.

Question 1: At what pressure will the stream come out as a saturated liquid at 390 $K$?

# Solution

- $x_k = z_k$
  Thus, $x_1 = 0.30,\ x_2 = 0.50,\ x_3 = 0.20$
- Compute vapor pressures from Antoine equation:

$$ln(P_1^0) = A_1 - \frac{B_1}{(C_1 + T)}$$

$$\Rightarrow P_1^0 = exp\left[A_1 - \frac{B_1}{(C_1 + T)}\right]$$

  Plugging in the values of $A_1, B_1, C_1$ we get
  $P_1^0 = 2084.87\ mm\ Hg$
  Similarly, we get $P_2^0 = 904.07\ mm\ Hg$ and
  $P_3^0 = 345.38\ mm\ Hg$.
- Choose toluene as the key component (as it is the most abundant).

- Average relative volatility is given by:

$$\begin{aligned}\bar{\alpha} &= \alpha_{1/2}x_1 + \alpha_{2/2}x_2 + \alpha_{3/2}x_3 \\ &= \frac{P_1^0}{P_2^0}x_1 + \frac{P_2^0}{P_2^0}x_2 + \frac{P_3^0}{P_2^0}x_3\end{aligned}$$

Substituting the values of vapor pressures and mole fractions, we get
$\alpha_{1/2} = 2.31, \qquad \alpha_{2/2} = 1, \qquad \alpha_{3/2} = 0.38$ and
$\bar{\alpha} = 2.31 \times 0.30 + 1 \times 0.50 + 0.38 \times 0.20 = 1.27$
The simplified bubble point equation (in terms of the key component) is given by $\frac{P_2^0}{P} = \frac{1}{\bar{\alpha}}$
Thus, the total pressure is given by $P = P_2^0\bar{\alpha}$
Substituting the values of $\bar{\alpha}$ and $P_2^0$, we get:
$P = 1148.17\ mm\ Hg$

What would be the answer if you chose benzene or o-xylene as the key component?

Question 2: At what pressure will the stream come out as a saturated vapor at 390 $K$?

- $y_k = z_k$
  Thus, $y_1 = 0.30, \; y_2 = 0.50, \; y_3 = 0.20$
- For calculating the pressure, we will use the dew point equation.

$$P = \frac{P_n^0}{\left( \sum \frac{y_k}{\alpha_{k/n}} \right)}$$

- We know $y_i$ from the feed composition and we already computed the values of the vapor pressure of toluene as well as the relative volatilities of benzene and o-xylene w.r.t. toluene in the previous slides.

- Substituting the values of $y_1, y_2, y_3$ from above and the values of $P_2^0$ and $\alpha_{1/2}, \alpha_{2/2}, \alpha_{3/2}$ computed earlier, we get

$$\begin{aligned} P &= \frac{904.07}{\left(\frac{0.3}{2.31} + \frac{0.5}{1} + \frac{0.2}{0.38}\right)} \\ &= 781.94 \, mm \; Hg \end{aligned}$$

- Note that at the same temperature, if the mixture comes out at as saturated vapor, the flash pressure is lower than when it comes out as saturated liquid.

Question 3: If the flash pressure is 1000 $mm\ Hg$ and the stream come out as a saturated liquid, what is the flash temperature?

- We use the bubble point equation in the following form:

$$P_n^0 = \frac{P}{\bar{\alpha}}$$

and the following iterative algorithm

1. Guess a temperature.
2. Compute $P_n^0$ and $\bar{\alpha}$ at this temperature.
3. Check if LHS = RHS. If the two sides of the equation are not equal, guess another temperature and go to step 2.

- Guess $T = 380\ K$
- Then, using the Antoine equation:
  $P_1^0 = 1620.39\ mm\ Hg,\ P_2^0 = 681.83\ mm\ Hg,$
  $P_3^0 = 250.71\ mm\ Hg$
- Thus,
  $$\bar{\alpha} = \frac{1620.39}{681.83} \times 0.30 + \frac{681.83}{681.83} \times 0.50 + \frac{250.71}{681.83} \times 0.20 = 1.29$$
- $LHS = P_2^0 = 681.83$
  $$RHS = \frac{P}{\bar{\alpha}} = \frac{1000}{1.29} = 775.19$$
- Since $LHS \neq RHS$ guess another temperature.

- Guess $T = 385\ K$
- Then, using the Antoine equation:
  $P_1^0 = 1841.50\ mm\ Hg,\ P_2^0 = 786.80\ mm\ Hg,$
  $P_3^0 = 294.99\ mm\ Hg$
- Thus, $\bar{\alpha} = 1.28$
- $LHS = P_2^0 = 786.80$
  $$RHS = \frac{P}{\bar{\alpha}} = \frac{1000}{1.28} = 781.25$$
- Since $LHS \approx RHS$ the guessed temperature of $385\ K$ is correct.
- Note that while $P_k^0$ varied substantially, $\bar{\alpha}$ did not vary much when a new temperature was guessed.

Question 4: If the flash pressure is 1000 $mm\ Hg$ and the stream come out as a saturated vapor, what is the flash temperature?

- We use the dew point equation in the following form:

$$P_n^0 = P\left(\sum \frac{y_k}{\alpha_{k/n}}\right)$$

and the following iterative algorithm

1. Guess a temperature.
2. Compute $P_n^0$ and $\alpha_{k/n}$ at this temperature.
3. Check if LHS = RHS. If the two sides of the equation are not equal, guess another temperature and go to step 2.

- Guess $T = 395\ K$
- Then, using the Antoine equation:
  $P_1^0 = 2351.87\ mm\ Hg,\ P_2^0 = 1034.61\ mm\ Hg,$
  $P_3^0 = 402.50\ mm\ Hg$
- Thus, $\alpha_{1/2} = 2.27,\ \alpha_{2/2} = 1,\ \alpha_{3/2} = 0.39$
- $LHS = P_2^0 = 1034.61$

$$RHS = P\left(\sum \frac{y_k}{\alpha_{k/n}}\right) = 1000\left(\frac{0.3}{2.27} + \frac{0.5}{1} + \frac{0.2}{0.39}\right)$$
$$= 1144.98$$

- Since $LHS \neq RHS$ guess another temperature.

- Guess $T = 399\ K$
- Then, using the Antoine equation:
  $P_1^0 = 2583.41\ mm\ Hg,\ P_2^0 = 1149.24\ mm\ Hg,$
  $P_3^0 = 453.44\ mm\ Hg$
- Thus, $\alpha_{1/2} = 2.25,\ \alpha_{2/2} = 1,\ \alpha_{3/2} = 0.39$
- $LHS = P_2^0 = 1149.24$

  $$RHS = 1000\left(\frac{0.3}{2.25} + \frac{0.5}{1} + \frac{0.2}{0.39}\right) = 1146.15$$
- Since $LHS \approx RHS$ the guessed temperature of $399\ K$ is correct.
- Note that while $P_k^0$ varied substantially, $\alpha_{k/n}$ did not vary much when a new temperature was guessed.

Question 5: If the flash pressure is 900 $mm\ Hg$ and the flash temperature is $390\ K$ what are the compositions of the vapor and liquid exiting the flash unit? What fraction of the feed is vaporized?

- Note that in this problem, the composition of the exiting streams need to be computed.
- Note that based on the answers of questions 1-4, we know that at the temperature and pressure given, part of the mixture is vapor and part of the mixture is liquid.

We will use the following iterative algorithm

1. Choose the key component $n$ and guess its split fraction, $\xi_n$.
2. Compute $\alpha_{k/n}$ at the flash temperature and compute the split fractions of the non-key components using the equation:

$$\xi_k = \frac{\alpha_{k/n}\xi_n}{1 + (\alpha_{k/n} - 1)\xi_n}$$

3. Compute the liquid and vapor flowrates from the split fractions.
4. Compute $x$ from the liquid flowrates and check the bubble point equation. If the bubble point equation is not satisfied, guess another split fraction and go to step 2.

- Choose toluene as the key component and guess $\xi_2 = 0.90$.
- Compute $\alpha_{1/2}$ and $\alpha_{3/2}$ at the given temperature.
  $P_1^0 = 2084.87\, mm\ Hg,\ P_2^0 = 904.07\, mm\ Hg,$
  $P_3^0 = 345.38\, mm\ Hg$
  Thus, $\alpha_{1/2} = 2.31$ and $\alpha_{3/2} = 0.38$
- The split fractions $\xi_1$ and $\xi_3$ are:

$$\begin{aligned}
\xi_1 &= \frac{2.31 \times 0.9}{1 + (2.31 - 1)0.9} \\
&= 0.95 \\
\xi_3 &= \frac{0.38 \times 0.9}{1 + (0.38 - 1)0.9} \\
&= 0.77
\end{aligned}$$

- Given the split fractions, the vapor and liquid flowrates can be computed.

$$v_1 = \xi_1 f_1 = 0.95 \times 30 = 28.5\ kmol/hr$$
$$v_2 = \xi_2 f_2 = 0.90 \times 50 = 45.0\ kmol/hr$$
$$v_3 = \xi_1 f_1 = 0.77 \times 20 = 15.4\ kmol/hr$$
$$l_1 = 30 - 28.5 = 1.5\ kmol/hr$$
$$l_2 = 50 - 45.0 = 5.0\ kmol/hr$$
$$l_3 = 20 - 15.4 = 4.6\ kmol/hr$$

- The total liquid flow = $1.5 + 5.0 + 4.6 = 11.1\ kmol/hr$
  Thus, the mole fractions in the liquid stream are:
  $$x_1 = \frac{1.5}{11.1} = 0.14, \quad x_2 = \frac{5}{11.1} = 0.45, \quad x_3 = \frac{4.6}{11.1} = 0.41$$

- Check the bubble point equation $P = \dfrac{\bar{\alpha}}{\alpha_{2/2}} P_2^0$

  $\bar{\alpha} = 0.14 \times 2.31 + 0.45 \times 1 + 0.41 \times 0.38 = 0.929$
  $LHS = 900\ mm\ Hg$
  $RHS = 0.929 \times 904.07 = 839.88\ mm\ Hg$

- Since $LHS \neq RHS$ the guessed split fraction of toluene ($\xi_2 = 0.9$) is incorrect and it is necessary to make another guess.

- Choose toluene as the key component and guess $\xi_2 = 0.65$.
- Compute $\alpha_{1/2}$ and $\alpha_{3/2}$ at the given temperature. Thus, $\alpha_{1/2} = 2.31$ and $\alpha_{3/2} = 0.38$
- The split fractions $\xi_1$ and $\xi_3$ are:

$$\begin{aligned}
\xi_1 &= \frac{2.31 \times 0.65}{1 + (2.31 - 1)0.65} \\
&= 0.81 \\
\xi_3 &= \frac{0.38 \times 0.65}{1 + (0.38 - 1)0.65} \\
&= 0.41
\end{aligned}$$

- Given the split fractions, the vapor and liquid flowrates can be computed.

$$
\begin{aligned}
v_1 &= \xi_1 f_1 = 0.81 \times 30 = 24.3\ kmol/hr \\
v_2 &= \xi_2 f_2 = 0.65 \times 50 = 32.5\ kmol/hr \\
v_3 &= \xi_1 f_1 = 0.41 \times 20 = 8.2\ kmol/hr \\
l_1 &= 30 - 24.3 = 5.7\ kmol/hr \\
l_2 &= 50 - 32.5 = 17.5\ kmol/hr \\
l_3 &= 20 - 8.2 = 11.8\ kmol/hr
\end{aligned}
$$

- The total liquid flow = $5.7 + 17.5 + 11.8 = 35\ kmol/hr$
  Thus, the mole fractions in the liquid stream are:
  $x_1 = \frac{5.7}{35} = 0.16, \quad x_2 = \frac{17.5}{35} = 0.50, \quad x_3 = \frac{11.8}{35} = 0.34$

- Check the bubble point equation $P = \frac{\bar{\alpha}}{\alpha_{2/2}} P_2^0$

$$\bar{\alpha} = 0.16 \times 2.31 + 0.50 \times 1 + 0.34 \times 0.38 = 0.999$$
$$LHS = 900\ mm\ Hg$$
$$RHS = 0.999 \times 904.07 = 903.16\ mm\ Hg$$

- Since $LHS \approx RHS$ the guessed split fraction of toluene ($\xi_2 = 0.65$) is correct.
- The vapor fraction can be computed as follows:

$$\begin{aligned} \text{Total moles of vapor} &= \text{Total feed - Total liquid} \\ &= 100 - 35 \\ &= 65\ kmol/hr \end{aligned}$$

Thus, $Vapor\ Fraction = \frac{65}{100} = 0.65$

Question 6: If the flash temperature is $390\ K$ and 60% of the feed is vaporized, what are the compositions of the vapor and liquid exiting the flash unit? What is the flash pressure?

- Guess the flash pressure to be $P = 900\ mm\ Hg$.
- Choose toluene as the key component and compute $K_n$ at the given temperature and guessed pressure.

  Thus, $K_2 = \dfrac{P_2^0}{P} = \dfrac{2084.87}{900} = 2.32$.
- Compute the key component split fraction $\xi_2$ from the equation:

$$\xi_n = \frac{1}{\dfrac{1}{K_n \phi} - \dfrac{1}{K_n} + 1}$$

Substituting $\phi = 0.60$ and $K_n = 2.32$ we get $\xi_2 = 0.77$

The rest of the solution is similar to that used for question 5.

- Compute $\alpha_{1/2}$ and $\alpha_{3/2}$ at the given temperatures and use these to compute split fractions $\xi_1$ and $\xi_3$ given $\xi_2$:
  $\alpha_{1/2} = 2.31$ and $\alpha_{3/2} = 0.38$
  $\xi_1 = 0.88$ and $\xi_3 = 0.56$
- Compute vapor and liquid flowrates

$$\begin{aligned}
v_1 &= \xi_1 f_1 = 0.88 \times 30 = 26.4 \; kmol/hr \\
v_2 &= \xi_2 f_2 = 0.77 \times 50 = 38.5 \; kmol/hr \\
v_3 &= \xi_3 f_3 = 0.56 \times 20 = 11.2 \; kmol/hr \\
l_1 &= 30 - 26.4 = 3.6 \; kmol/hr \\
l_2 &= 50 - 38.5 = 11.5 \; kmol/hr \\
l_3 &= 20 - 11.2 = 8.8 \; kmol/hr
\end{aligned}$$

- Compute liquid mole fractions and average relative volatility.
  $x_1 = 0.15, \quad x_2 = 0.48, \quad x_3 = 0.37$
  $\bar{\alpha} = 2.28 \times 0.15 + 1 \times 0.48 + 0.38 \times 0.37 = 0.963$

- Check bubble point equation $P = \bar{\alpha} P_2^0$.
  $LHS = 900\ mm\ Hg$ (guessed value)
  $RHS = 0.963 \times 904.07 = 870.62\ mm\ Hg$
- $LHS \neq RHS$ and thus the guessed pressure is wrong.
- Guess another pressure and iterate.

How would you solve the problem if the pressure was given but the temperature was not given.

| | |
|---|---|
| √ $T_V,\ P_V$ specified | Isothermal flash |
| √ $V/F = 0,\ P_L$ specified | Bubble point temperature |
| √ $V/F = 1,\ P_V$ specified | Dew point temperature |
| √ $T_L$ specified, $V/F = 0$ | Bubble point pressure |
| √ $T_V$ specified, $V/F = 1$ | Dew point pressure |
| $Q = 0,\ P_V$ specified | Adiabatic flash |
| $Q, P_V$ specified | Nonadiabatic flash |
| √ $V/F,\ P_V$ specified | Percent vaporization flash |

Adiabatic and non-adiabatic flash will be covered in the "Energy Balance" lecture.