

Mass Transfer Operations-I
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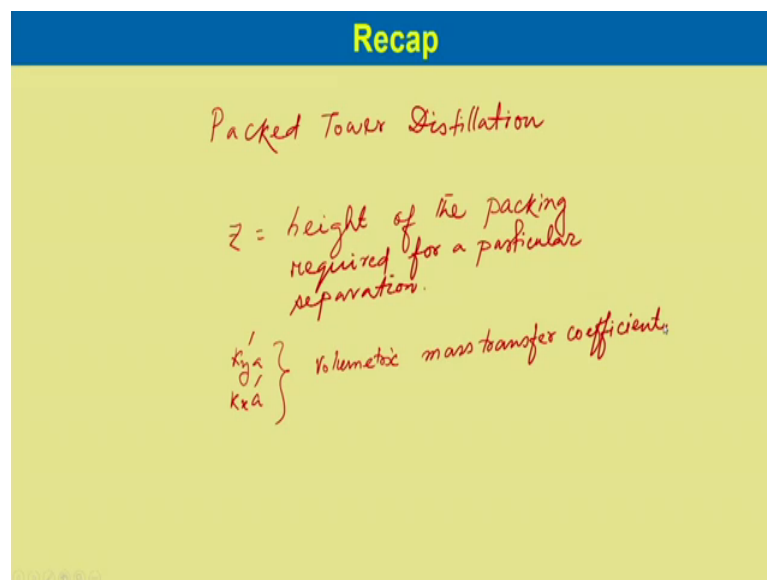
Distillation-V

Lecture - 39

Introduction to multicomponent distillation and multicomponent flash distillation

Welcome to the 14th lecture of module 5 of Mass Transfer Operation; in this module we are discussing distillation operation. Before going to this lecture let us have a brief recap on our previous lecture, on our previous lecture we have mainly considered one important topic is the packed tower distillation.

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In the packed tower distillation we have seen what are the types of liquid mixtures we can use for packed tower distillation and what would be the conditions of those liquid mixtures, at the same time we have considered to calculate the height of the tower required that is z and we have seen that it is similar to the packed tower absorption operations. And we have considered the packed tower design based on the volumetric mass transfer coefficient both in the liquid phase as well as in the gas phase that is, $K_y a$ and $K_x a$.

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Module 5: Lecture 14

Multi-component Distillation

- (1) Bubble point & Dew point calculation
- (2) Multi-component flash distillation
- (3) Multi-component Batch distillation
- (4) Minimum Number of plates
- (5) Minimum Reflux
- (6) Approximate method to calculate vapour and liquid composition.

So, in this lecture we will consider multicomponent distillation, under which we will mainly focus on bubble point and dew point calculation. The second thing we will consider is the multicomponent flash distillation, then we will consider multicomponent batch distillation, we will also consider to find out the minimum number of plates that is a total reflux. So, then we will consider minimum reflux and finally, we will consider the approximate method or Underwood method to calculate the compositions of the tower and the number of trays required.

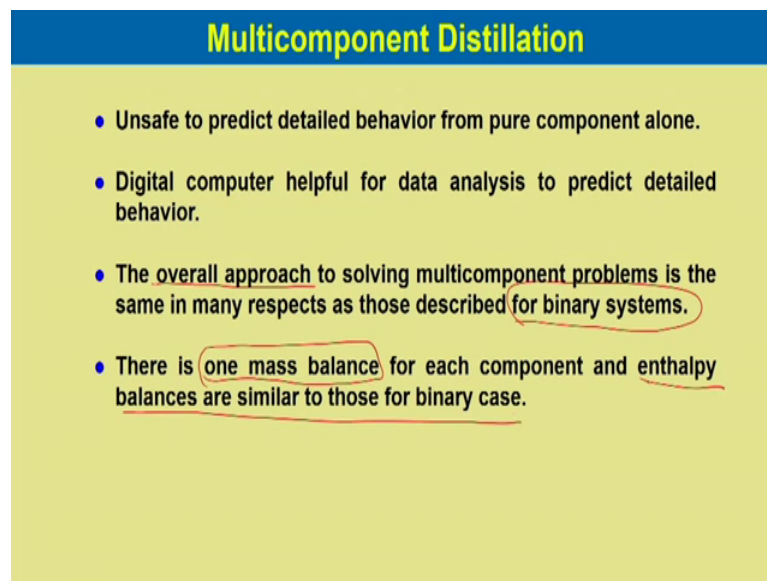
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Multi-component Distillation

- **Three component system**
 - ✓ Graphical treatment possible using triangular diagram
- **More than three components**
 - ✓ Graphical treatment very complicated
- **For practical application**
 - ✓ Liquid phase may be assumed ideal
 - ✓ Roult's law applicable
 - ✓ Equilibrium data can be obtained from pure component

So, multicomponent distillation, so there are three component systems at least more than two component systems if it is three component systems, then graphical treatment is possible using triangular diagram. If more than three components are there in that case graphical treatment is very complicated. For practical application liquid phase may be assumed ideal, Raoult's law may be applicable and equilibrium data can be obtained from pure component data.

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Multicomponent Distillation

- Unsafe to predict detailed behavior from pure component alone.
- Digital computer helpful for data analysis to predict detailed behavior.
- The overall approach to solving multicomponent problems is the same in many respects as those described for binary systems.
- There is one mass balance for each component and enthalpy balances are similar to those for binary case.

Now, it is unsafe to predict detailed behaviour from pure component alone. So, digital computer is helpful for data analysis to predict detail behaviour. The overall approach to solving multicomponent problems is the same in many respect as those described for binary systems. So, if we consider overall approach for the solution of the multicomponent systems or for the design of the multicomponent systems, in many respect it will be similar as those we have considered for the binary system.

There is one mass balance for each component and enthalpy balances are similar to those for binary case. So, what we can see? Here in this case the mass balance for each component will be one for each component we will have one mass balance and the enthalpy balance would be similar to those for the binary case.

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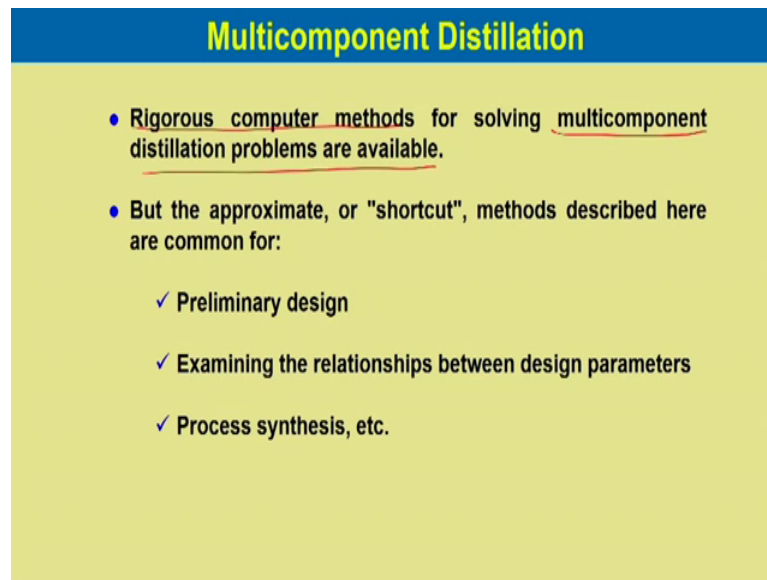
Multicomponent Distillation

- The equilibrium relationships are more complex for multicomponent systems.
- In particular, the identity of the most volatile component may change with temperature in the system.
- Equilibrium data are used to calculate multicomponent bubble and dew points.
- The limiting cases of total and infinite reflux apply to multicomponent columns just as they do to binary systems.

The equilibrium relationships are more complex for multicomponent systems. In particular, the identity of the most volatile component may change with temperature of the systems. Please note that the identity of the most volatile component may change with temperature of the system.

Equilibrium data are used to calculate multicomponent bubble and dew points. The limiting cases of total and infinite reflux applied to multicomponent columns just as they do for the binary systems. So, in this case also we can apply the limiting cases for total reflux and infinite reflux and that would be similar as we do for the binary systems.

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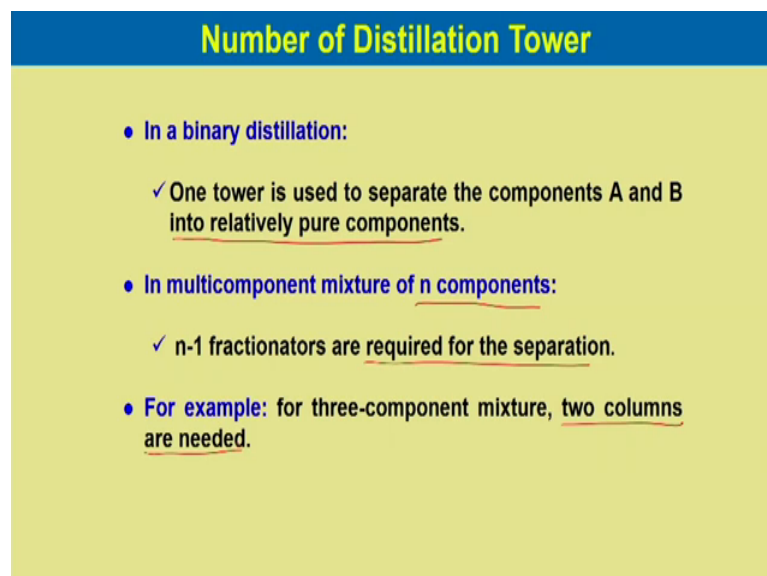
Multicomponent Distillation

- Rigorous computer methods for solving multicomponent distillation problems are available.
- But the approximate, or "shortcut", methods described here are common for:
 - ✓ Preliminary design
 - ✓ Examining the relationships between design parameters
 - ✓ Process synthesis, etc.

Now, rigorous computer methods for solving multicomponent distillation problems are available. But the approximate or shortcut methods described here are common for preliminary design, examining the relationship between the design parameters and process synthesis etcetera.

Although there are rigorous method, computer methods available for the multicomponent distillation problems, but approximate method can be helpful for preliminary design, examining the relationship between the design parameters process synthesis and so on.

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Number of Distillation Tower

- **In a binary distillation:**
 - ✓ One tower is used to separate the components A and B into relatively pure components.
- **In multicomponent mixture of n components:**
 - ✓ n-1 fractionators are required for the separation.
- **For example:** for three-component mixture, two columns are needed.

Now, number of distillation tower in a binary distillation as we know one tower is used to separate the components A and B into relatively pure components. So, we generally use one tower having several trays which can separate the binary component into fractions relatively pure component fractions.

But in multicomponent mixture of n components we need n minus 1 fractionators which are required for the separation. That means, if we have three component mixture, then n is equal to three, so we need n minus one fractionator; that means, two columns are needed.

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Design Calculation Method

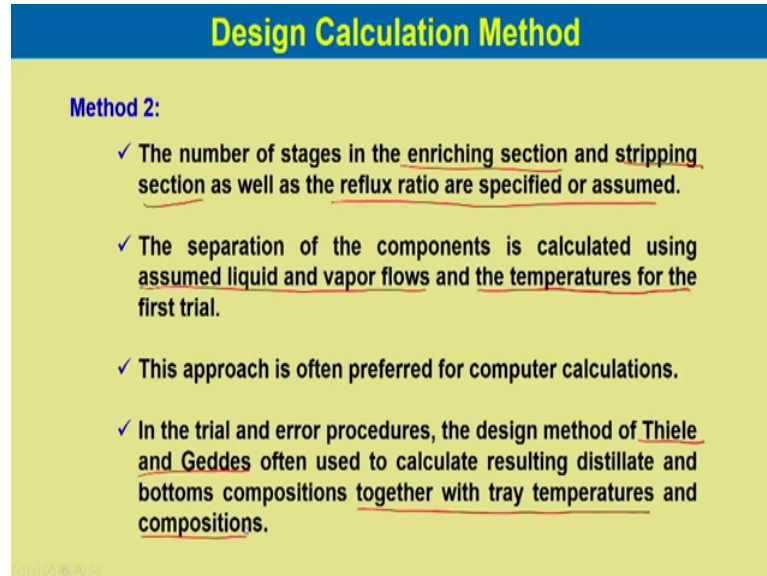
- In a design, the conditions of the feed are generally known or specified (temperature, pressure, composition, flow rate).
- The calculation procedure follows two general methods.
- **Method 1:**
 - ✓ The desired separation or split between two of the components is specified and the number of theoretical stages is calculated for a selected reflux ratio.
 - ✓ It is clear that with more than two components in the feed, the complete compositions of the distillate and bottoms are not known, then trial and error procedures must be used.

In a design the conditions of the feed are generally known or specified; that means, the temperature, pressure, composition and flow rate this conditions of the feed are generally known or it should be specified at the beginning of the design. The calculation procedure follows two general method let us consider what are those. Method 1 the desired separation or split between two of the components is specified and the number of theoretical stages is calculated for a selected reflux ratio.

So, the split or separation between the two components has to be specified and then we calculate the number of theoretical stages based on a selected reflux ratio. It is clear that with more than two components in the feed, the complete composition of the distillate and the bottoms are not known, then trial and error procedure must be used. This is very clear for more than two component systems in the feed, the complete composition of the

distillate and bottoms are not known. So, we should follow the trial and error procedure to calculate the compositions.

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Design Calculation Method

Method 2:

- ✓ The number of stages in the enriching section and stripping section as well as the reflux ratio are specified or assumed.
- ✓ The separation of the components is calculated using assumed liquid and vapor flows and the temperatures for the first trial.
- ✓ This approach is often preferred for computer calculations.
- ✓ In the trial and error procedures, the design method of Thiele and Geddes often used to calculate resulting distillate and bottoms compositions together with tray temperatures and compositions.

Method 2: the number of stages in the enriching section and stripping section as well as the reflux ratio are specified or assumed. So, both section enriching section and stripping section in addition to that the reflux ratio has to be specified at the beginning. The number of component is calculated using assumed, liquid and vapour flows and the temperature for the first trial.

So, what we are assuming liquid and vapour flows and the temperature for the first trial, this approach is often preferred for computer calculation. In the trial and error procedures the design method of Thiele and Geddes is often used to calculate the resulting distillate and bottoms composition together with tray temperature and compositions.

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Equilibrium in Multicomponent Systems

- Experimental VLE data not known in most multicomponent system.
- Generally computed from available equations or correlations.
- Ideal behavior may be assumed so that Roult's law is applicable.
- Hydrocarbons of a homologous series form nearly ideal solutions.

Now, equilibrium in multicomponent systems experimental VLE data not known in most multicomponent system; generally computed from available equations or correlations. Ideal behaviour may be assumed, so that we can apply the Roult's law. Hydrocarbons of a homologous series from nearly ideal solutions we have earlier discussed what are the conditions requires for an ideal solutions and we have seen that hydrocarbons of homologous series they form nearly ideal solutions.

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Equilibrium in Multicomponent Systems

- Now:
$$y_j P_j = p_j^* = x_j P_j^* \quad \text{and} \quad P_j = \sum_{i=1}^n p_i^* \quad \text{1}$$

$$\Rightarrow y_j = \frac{p_j^*}{P_j} = \frac{x_j P_j^*}{\sum_{i=1}^n p_i^*} \quad \text{2}$$
- Where: P_j^* = vapor pressure of component j at the given temperature
- At a given temperature, the vapor pressures of the components are known.
- Therefore for a particular liquid composition, the vapour compositions can be calculated. ✓

We know that $y_j^* P_t$ would be equal to $P_j^* x_j$ is the mole fractions of component j into P_t is the total pressure is equal to P_j^* is the partial pressure of component j which we can write x_j into $P_j^* x_j$ is the mole fractions of component j in the liquid phase and P_j^* is the vapour pressure of component j and P_t we can write summation over i is equal to 1 to n P_i^* . That is partial pressure or the components, so this is equation 1.

Now if we rearrange these equations we can write y_j^* would be equal to $P_j^* x_j$ by P_t . So, P_t as we know it is summation over i is equal to 1 to n P_i^* , so, we can substitute here in this case is summation over i is equal to one to n P_i^* and this is nothing, but $x_j P_j^*$ divided by summation over i is equal to 1 to n P_i^* . So, this is equation 2.

Where P_j^* as I have said before it is vapour pressure of component j at the given temperature. At a given temperature the vapour pressure of the components are known. Therefore, for a particular liquid composition, the vapour composition can be calculated.

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Equilibrium in Multicomponent Systems

- **Noting:** $\alpha_j = \frac{P_j^*}{P_j^*}$

$y_j^* = \frac{P_j^*}{P_t} = \frac{x_j P_j^*}{\sum_{i=1}^n P_i^*}$
2

- **Eq. (2) can be rewritten as:**

$$y_j^* = \frac{x_j P_j^*}{\sum_{i=1}^n x_i P_i^*}$$

3

- **Once the equilibrium vapor phase mole fractions are known, the partial pressures and the total pressures can be calculated from eq. (1)**

$$y_j^* P_t = P_j^* x_j \quad \text{and} \quad P_t = \sum_{i=1}^n P_i^* x_i$$

1

Now, if we define α_{ij} is equal to P_i^* divided by P_j^* here α_{ij} is the relative volatility of component i with respect to j that is vapour pressure of component i divided by the vapour pressure of component j. So, in that case we can write this equation over here as y_j^* would be equal to x_j divided by $\sum_{i=1}^n \alpha_{ij} x_i$

to $n \times i \times P_i^v$. Once the equilibrium vapour phase mole fractions are known, the partial pressure and the total pressure can be calculated from equation 1.

So, if we can calculate the equilibrium vapour pressure, equilibrium vapour phase mole fractions then and the partial pressure as well as the total pressure can be calculated from this equation. So, which is shown before that is $y_j^* \text{ into } P_t$ is equal to P_j^* is equal to $x_j \times P_j^v$ and P_t would be equal to summation over i is equal to 1 to $n \times P_i^*$.

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Equilibrium in Multicomponent Systems

- For multicomponent systems, the equilibrium data is described by means of distribution coefficient, m .
- For component j : $\Rightarrow m_j = \frac{y_j^*}{x_j}$ 4 ✓
- where in general, m_j depends upon the temperature, pressure and composition of the mixture.
- The relative volatility of component i w.r.t j in multicomponent mixture is defined by:

$$\Rightarrow \alpha_{ij} = \frac{y_i^*/x_i}{y_j^*/x_j} = \frac{m_i}{m_j}$$
 5

For multi component systems, the equilibrium data is described by means of distribution coefficient which is m . For component j we can write m_j is equal to y_j^* divided by x_j , so this is defined by equation 4; where in general m_j depends upon the temperature, pressure and composition of the mixture.

The relative volatility of component i with respect to j in multi component mixture is defined by α_{ij} is equal to y_i^* divided by x_i divided by y_j^* by x_j as we have seen before from equation 1 it is the $y_j^* \text{ into } P_t$ is equal to $x_i \text{ into } x_j \text{ into } P_j^v$ the vapour pressure of component v . So, if we substitute over here we will get this as m_j divided by m_i divided by m_j this is equation 5.

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Equilibrium in Multicomponent Systems

- For ideal solutions at moderate pressure, m_j is independent of composition and depends upon the temperature (as this affect vapor pressure) and the total pressure.
- Therefore:

$$m_j = \frac{P_j^v}{P_t} \quad 6$$
$$\alpha_{ij} = \frac{P_i^v}{P_j^v} \quad 7$$

For ideal solutions at moderate pressure, m_j is independent of composition and depends upon the temperature, as this affect vapour pressure and the total pressure. So, if we consider ideal solution at moderate pressure in that case m_j we can consider as independent of the composition, but it will depend upon the temperature and the total pressure therefore, we can write m_j is equal to P_j^v divided by P_t . So, α_{ij} is equal to P_i^v divided by P_j^v .

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Bubble Point Calculations

- For bubble point vapor:

$$\sum y_i^* = 1.0$$
$$\text{or } m_A x_A + m_B x_B + m_C x_C + \dots = 1.0 \quad 8$$

- For component J as reference component:

$$\frac{m_A x_A}{m_j} + \frac{m_B x_B}{m_j} + \frac{m_C x_C}{m_j} + \dots = \frac{1.0}{m_j}$$
$$\text{or } \alpha_{AJ} x_A + \alpha_{BJ} x_B + \alpha_{CJ} x_C + \dots = \sum \alpha_{iJ} x_i = \frac{1}{m_j} \quad 9$$

Now, bubble point calculations for bubble point calculations we know that summation over y_i that is summation over all the mole fractions in the vapour phase would be equal to 1. So, or we can write m_A into x_A plus m_B into x_B plus m_C into x_C plus so on up to the n th component would be equal to 1, so, this is equation 8.

Now for component j as the reference component we can divide this equation with m_j , so if we divide with m_j , so then this equations would become $m_A x_A$ divided by m_j plus $m_B x_B$ divided by m_j plus $m_C x_C$ divided by m_j and so on and would be equal to 1 by m_j .

Now, m_A by m_j is nothing, but $\alpha_{A,j}$ that is the relative volatility of component A with respect to J . So, similarly we can write $\alpha_{A,j} x_A$ plus $\alpha_{B,j} x_B$ plus $\alpha_{C,j} x_C$ and so on. So, this we can write summation over $\alpha_{i,j} x_i$ would be equal to 1 by m_j , so this is equation 9.

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Bubble Point Calculations

- Bubble point vapor composition is given by:

$$y_i = \frac{\alpha_{i,j} x_i}{\sum \alpha_{i,j} x_i}$$
10 ✓
- The liquid composition and total pressure is fixed, the calculation of temperature is made by trial and error to satisfy equation (8).

$$\sum y_i^* = 1.0$$
 or $m_A x_A + m_B x_B + m_C x_C + \dots = 1.0$
8 ✓

Bubble point vapour composition is given by y_i which is equal to $\alpha_{i,j} x_i$ divided by summation over $\alpha_{i,j} x_i$ this is equation 10. The liquid composition and total pressure is fixed, the calculation of temperature is made by trial and error to satisfy equation 8. So, this is equation 8, so trial and error method has to be followed to satisfy this equation.

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Dew Point Calculations

- For the dew point liquid:

$$\sum x_i = 1.0$$

$$\frac{y_A}{m_A} + \frac{y_B}{m_B} + \frac{y_C}{m_C} + \dots = 1.0 \quad \text{11}$$
- For component J as reference component:

$$\frac{m_J y_A}{m_A} + \frac{m_J y_B}{m_B} + \frac{m_J y_C}{m_C} + \dots = 1.0 \times m_J$$
 or,
$$\frac{y_A}{\alpha_{AJ}} + \frac{y_B}{\alpha_{BJ}} + \frac{y_C}{\alpha_{CJ}} + \dots = \sum y_i / \alpha_{iJ} = m_J \quad \text{12}$$
- Equilibrium dew point vapor composition is given by:

$$x_i = \frac{y_i / \alpha_{iJ}}{\sum y_i / \alpha_{iJ}} \quad \text{13}$$

For the dew point liquid summation over x i would be equal to 1 and y A by m A plus y B by m B plus y C by m C and so on would be equal to 1. Now for component J as reference component we can multiply with m J both the sides, so it would be into m J. So, here we can write y A divided by alpha AJ plus y B by alpha BJ plus y C by alpha CJ and so on which would be equal to summation over y J by alpha i J would be equal to m J, so this is equation 12 for dew point calculation.

Equilibrium dew point vapour composition is given by x i would be equal to y i divided by alpha i J divided by summation over y i by alpha i J, so this is equation thirteen. So, for bubble point and dew point we know the equilibrium composition vapour and liquid composition calculation and also we know the distribution coefficient how to calculate.

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Example 1

A solution of hydrocarbons at a total pressure of 350 kN/m² contains 5mol% n-C₃H₈, 30mol% n-C₄H₁₀, 40mol% n-C₅H₁₂ and 25 mol% n-C₆H₁₄. Compute the bubble point and dew point.

So, now, we will proceed with an example to see how to calculate bubble point and dew point. A solution of hydrocarbons at a total pressure of 350 kilo Newton per meter square contains 5 mole percent propane normal propane, 30 mole percent normal butane, 40 mole percent normal pentane and 25 mole percent normal hexane. Now we need to calculate the bubble point and dew point.

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Example 1: Solution

A solution of hydrocarbons at a total pressure of 350 kN/m² contains 5mol% n-C₃H₈, 30mol% n-C₄H₁₀, 40mol% n-C₅H₁₂ and 25 mol% n-C₆H₁₄. Compute the bubble point and dew point.

Solution:

- The values of m_i will be taken from nomograph, which assumed ideal liquid solutions.

Bubble Point Calculation

| i Col 1 | x_i Col 2 | m_i 60°C Col 3 | α_{i,C_3} Col 4 | $\alpha_{i,C_3} x_i$ Col 5 | m_i 56.8°C Col 6 | α_{i,C_3} Col 7 | $\alpha_{i,C_3} x_i$ Col 8 | y_i Col 9 |
|------------------|----------------|------------------------|---------------------------|-------------------------------|--------------------------|---------------------------|-------------------------------|----------------|
| n-C ₃ | 0.05 | 4.70 | 7.58 | 0.379 | 4.60 | 7.82 | 0.391 | 0.229 |
| n-C ₄ | 0.30 | 1.70 | 2.74 | 0.822 | 1.60 | 2.72 | 0.816 | 0.478 |
| n-C ₅ | 0.40 | 0.62 | 1.00 | 0.400 | 0.588 | 1.00 | 0.400 | 0.234 |
| n-C ₆ | 0.25 | 0.25 | 0.403 | 0.1008 | 0.235 | 0.40 | 0.100 | 0.0586 |

The values of m which can be taken from monograph and which assumed ideal liquid solution. So, we have considered ideal liquid solution and the values of m , the

distribution coefficient can be taken from the monograph. Now, for bubble point calculations we will obtain a table like this and we will go step by step how to obtain this table?

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Example 1: Solution

A solution of hydrocarbons at a total pressure of 350 kN/m² contains 5mol% n-C₃H₈, 30mol% n-C₄H₁₀, 40mol% n-C₅H₁₂ and 25 mol% n-C₆H₁₄. Compute the bubble point and dew point.

Solution: Steps

| i Col 1 | x_j Col 2 | m_i 60°C Col 3 | α_{i,C_5} Col 4 | $\alpha_{i,C_5} x_j$ Col 5 | m_i 56.8°C Col 6 | α_{i,C_5} Col 7 | $\alpha_{i,C_5} x_j$ Col 8 | y_i Col 9 |
|------------------|----------------|------------------------|---------------------------|-------------------------------|--------------------------|---------------------------|-------------------------------|----------------|
| n-C ₃ | 0.05 | 4.70 | 7.58 | 0.379 | 4.60 | 7.82 | 0.391 | 0.229 |
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- First estimate of BP, 60°C is chosen. Col3 list corresponding m's at 60°C, 350 kN/m²
- Reference component is chosen to be pentane and Col4 list the relative volatility ($\alpha_{C_3,C_5} = 4.70 / 0.62 = 7.58$ etc)

First we need to estimate of bubble point that is 60 degree Centigrade is chosen and column three over here, so with respect to 60 degree, the corresponding and the pressure we know 350 kilo Newton per meter square. So, the reference component is chosen to be pentane and column 4 list the relative volatility.

In this case you can see the relative volatility that is with respect to the component 5 which is the reference component. So, alpha i C 5 is the relative volatility of component i with respect to component 5. So, initially 60 degree temperature is chosen and the data for the distribution coefficient is taken from the literature and then we have calculated these are the mole fractions given in the problems, that is 5 mole percent normal propane.

And then, 30 mole percent is normal butane which is here 40 mole percent normal pentane and 25 mole percent normal hexane. So, these are given first column represents the component, second column represents the mole fractions and the third column which represents the distribution coefficient and we have assumed the temperature 60 degree Centigrade

And then we can obtain the distribution coefficient from the monograph, column 4 you can see is the relative volatility and which can be calculated with respect to the reference component which is 0.62 one calculation is shown over here. In this case 4.70 for normal propane and for normal pentane it is 0.62, so we can write 0.7 naught divided by 0.62, so this is 7.54 which is written over here. Similar for the other case we can also calculate in this table

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Example 1: Solution

A solution of hydrocarbons at a total pressure of 350 kN/m² contains 5mol% n-C₃H₈, 30mol% n-C₄H₁₀, 40mol% n-C₅H₁₂ and 25 mol% n-C₆H₁₄. Compute the bubble point and dew point.

Solution: Steps

| i | x_i | m_i 60°C | α_{i,C_3} | $\alpha_{i,C_3} x_i$ | m_i 56.8°C | α_{i,C_3} | $\alpha_{i,C_3} x_i$ | y_i |
|------------------|-------|---------------|------------------|----------------------|-----------------|------------------|----------------------|--------|
| Col 1 | Col 2 | Col 3 | Col 4 | Col 5 | Col 6 | Col 7 | Col 8 | Col 9 |
| n-C ₃ | 0.05 | 4.70 | 7.58 | 0.379 | 4.60 | 7.82 | 0.391 | 0.229 |
| n-C ₄ | 0.30 | 1.70 | 2.74 | 0.822 | 1.60 | 2.72 | 0.816 | 0.478 |
| n-C ₅ | 0.40 | 0.62 | 1.00 | 0.400 | 0.588 | 1.00 | 0.400 | 0.234 |
| n-C ₆ | 0.25 | 0.25 | 0.403 | 0.1008 | 0.235 | 0.40 | 0.100 | 0.0586 |

$\Sigma \alpha_{i,C_3} x_i = 1.702$

- $\Sigma \alpha_{i,C_3} x_i = 1.702$ In Col5, whereas $m_{C_5} = 1/1.702 = 0.588$. $m_j = \frac{1}{\Sigma \alpha_{i,j} x_i}$
- Corresponding temperature from the monograph is 56.8°C.

Now, summation over all the components over here in column 5 we can calculate the sum over here which is summation of all these it will give about 1.702. Now we know that m_j is equal to 1 by summation over $\alpha_{i,j} x_i$. So, this $\alpha_{i,j} x_i$, that is $\alpha_{i,C_3} x_i$ summation over $\alpha_{i,C_3} x_i$ is equal to 1.702, so 1 by that values would give us m_{C_5} which is m_j . So, m_{C_5} is 0.588, so we can calculate this.

Now, with respect to this distribution coefficient values corresponding temperature can be obtained from the monograph, so which is shown over here. So, we can calculate this temperature based on this data distribution coefficient data. Once we obtained this temperature from the monograph we can calculate the distribution coefficient of other component at that temperature and the pressure mentioned. So, which is shown over here it is 56.8 degree Centigrade.

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Example 1: Solution

A solution of hydrocarbons at a total pressure of 350 kN/m² contains 5mol% n-C₃H₈, 30mol% n-C₄H₁₀, 40mol% n-C₅H₁₂ and 25 mol% n-C₆H₁₄. Compute the bubble point and dew point.

Solution: Steps

| i Col 1 | x_i Col 2 | m_i 60°C Col 3 | α_{i,C_3} Col 4 | $\alpha_{i,C_3} x_i$ Col 5 | m_i 56.8°C Col 6 | α_{i,C_3} Col 7 | $\alpha_{i,C_3} x_i$ Col 8 | y_i Col 9 |
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| n-C ₅ | 0.40 | 0.62 | 1.00 | 0.400 | 0.588 | 1.00 | 0.400 | 0.234 |
| n-C ₆ | 0.25 | 0.25 | 0.403 | 0.1008 | 0.235 | 0.40 | 0.100 | 0.0586 |

- The calculations are repeated for this temperature in Col6 to Col8.
- $m_{C_5} = 1/1.707 = 0.586$, corresponding to $t = 56.7^\circ\text{C}$, which is nearly equal to 56.8 (assumed)
- This is the bubble point temperature. And corresponding vapor composition is given in Col9 ($0.391/1.707 = 0.229$)

Now the calculation are repeated for this temperature in column 6 to column 8. So, similar to the earlier one 6 at this temperature once this is known we can calculate the summation of this and which would be 1.707 and with respect to that we can calculate m_{C_5} which is 0.586 which is written over here and which is close to this temperature and corresponding to that we have 56.7 degree Centigrade which is nearly equal to the 56.8 assumed.

So, further calculation has not been done based on that this has been calculated. So, this is how we can obtain the bubble point temperature, this is the bubble point temperature and corresponding vapour composition is given in column 9 over here which is 0.229 and we can calculate the other compositions

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Example 1: Solution

A solution of hydrocarbons at a total pressure of 350 kN/m² contains 5mol% n-C₃H₈, 30mol% n-C₄H₁₀, 40mol% n-C₅H₁₂ and 25 mol% n-C₆H₁₄. Compute the bubble point and dew point.

Solution: Steps

Dew Point Calculation

- Assume 80°C, when $\sum \frac{y_i}{\alpha_{i,C_5}} = 1.081 = m_{C_5}$,

| i | y _i | m _i 80°C | α _{i,C₅} | y _i /α _{i,C₅} | m _i 83.7°C | α _{i,C₅} | y _i /α _{i,C₅} | x _i |
|------------------|----------------|------------------------|------------------------------|--|--------------------------|------------------------------|--|----------------|
| Col1 | Col2 | Col3 | Col4 | Col5 | Col6 | Col7 | Col8 | Col9 |
| n-C ₃ | 0.05 | 6.30 | 6.56 | 0.80762 | 6.60 | 6.11 | 0.00818 | 0.0074 |
| n-C ₄ | 0.30 | 2.50 | 2.60 | 0.1154 | 2.70 | 2.50 | 0.120 | 0.1088 |
| n-C ₅ | 0.40 | 0.96 | 1.0 | 0.400 | 1.08 | 1.00 | 0.40 | 0.3626 |
| n-C ₆ | 0.25 | 0.43 | 0.448 | 0.558 | 0.47 | 0.435 | 0.575 | 0.5213 |

- T=83.7°C repetition lead to m_{C₅}=1.103 corresponding to 84°C, which in the dew point.

Now, we will consider the dew point calculation. So, for dew point calculations similar to the bubble point calculations we will follow the calculation procedure in case of the dew point calculation. Now we need to assume a temperatures say 80 degree centigrade temperature then we can calculate y_i by alpha_{i,5}, so, which is over here which is 1.081. So, like the bubble point in case of the dew point we have to assume the temperature, at that temperature we have to calculate the distribution coefficient once this is noted we can calculate the relative volatility with respect to this.

And then once this relative volatility is obtained we can divide the mole fractions with the relative volatility and we can obtain the data as shown in column 5. So, once this is obtained, then we can see the temperature is 83.7 which is obtained corresponding to the values of 1.081 which is shown over here.

So, corresponding to this distribution coefficient values we can choose the temperature and then we can calculate the other distribution coefficient and this process is repeated and shown in the other columns and it was seen that the temperature which was obtained is close to the assumed temperature in this case so that is 83.7. So, this is the dew point temperature.

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Multicomponent Flash Distillation

- Fraction of feed vaporized $f = V/F$ ✓
- Fraction of feed remaining as liquid $(1-f) = L/F$ ✓
- Component i balance: $y_i = \frac{f-1}{f} x_i + \frac{x_{if}}{f}$ ✓

Where:

y_i is the composition of i in the vapour, in equilibrium with x_i in the liquid after vaporization. ✓

Now, we will consider multi component flash distillation, as we have defined before in case of the flash distillation, the fraction of the feed vaporized f is equal to V by F , the small f is equal to V by F . Fraction of the feed remaining as liquid is 1 minus f which is equal to L by F .

Now if we do the balance on component i we can write y_i is equal to f minus 1 divided by f into x_i plus $x_i f$ divided by f . So, $x_i f$ is the feed composition or feed concentration of component i , y_i is the composition of i in the vapour in equilibrium with x_i which is in the liquid after vaporization, so this is equation 14.

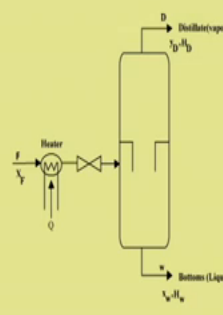
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Multicomponent Flash Distillation

- Because a flash is a single equilibrium stage, equilibrium fixes another relationship between y and x.
- Combining equilibrium and operating equations

$$y_i = K_i x_i = K_c \alpha_i x_i, \text{ when } \alpha_i = K_i / K_c$$
- Now, component balance equation becomes

$$y_i = K_c \alpha_i x_i = \frac{f-1}{f} x_i + \frac{x_{iF}}{f}$$



Now, because a flash is a single equilibrium stage equilibrium fixes another relationship between y and x. Combining equilibrium and operating equations that is y_i is equal to $K_i x_i$ is equal to $K_c \alpha_i x_i$ where α_i is K_i by K_c ; K_c is the equilibrium constant and K_i is the distribution coefficient. So, now, the component balance equations we can write y_i is equal to $K_c \alpha_i x_i$ which would be equal to $\frac{1-f}{f} x_i + \frac{x_{iF}}{f}$, so this is equation 15.

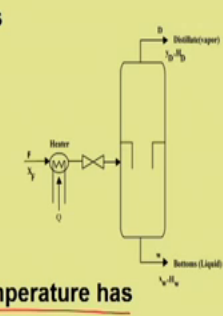
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Multicomponent Flash Distillation

- Solving for x_i and summing for all components

$$\sum x_i = \sum \frac{x_{iF}}{f(K_c \alpha_i - 1) + 1} = 1.0$$
- Solved by trial and error by first assuming a temperature if the fraction f vaporized has been set.
- When the $\sum x_i$ values add up 1.0, the proper temperature has been chosen.
- The composition of the vapor y_i can be obtained from:

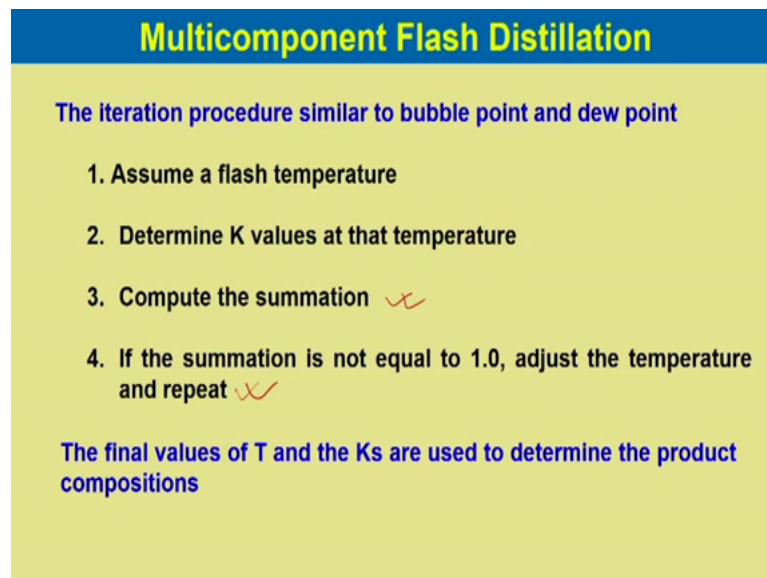
$$y_i = K_c \alpha_i x_i$$
 Or by a material balance.



Now, solving for x_i and summing for all components if we do that summation over x_i would be equal to summation over $x_i f$ divided by f into $K_c \alpha_i - 1 + 1$ is equal to 1.0 because the summation over all component is equal to 1. Solve by trial and error by first assuming a temperature if the fraction f vaporized has been set. So, we can set the fraction vaporized which is f , then we can assume a temperature and then solve by trial and error.

When the summation over x_i values add up to 1, the proper temperature has to be chosen. The composition of the vapour that is y_i can be obtained from y_i is equal to $K_c \alpha_i x_i$. So, once that is temperature is obtained then we can obtain the composition of the vapour using this relation or we can do by a material balance relations.

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Multicomponent Flash Distillation

The iteration procedure similar to bubble point and dew point

1. Assume a flash temperature
2. Determine K values at that temperature
3. Compute the summation ✓
4. If the summation is not equal to 1.0, adjust the temperature and repeat ✓

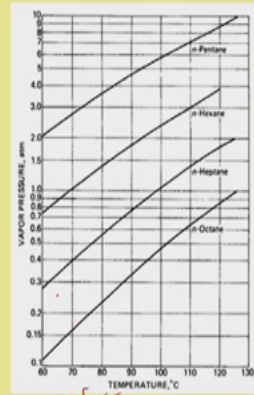
The final values of T and the Ks are used to determine the product compositions

The iteration procedure similar to bubble point and dew point for this multicomponent flash distillation; so, what we need to do? We need to assume a flash temperature, determine K values at that temperature and then compute the summation. If the summation is not equal to 1 adjust the temperature and repeat. The final values of T and the Ks are used to determine the product composition.

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Example 2

A mixture of hydrocarbons containing 32 mole% n-hexane, 38 mole% n-heptane and 30 mole% n-octane is subjected to a flash distillation at 1.2 atm pressure and 40% of the feed is vaporized. Find the temperature of the flash and the composition of the liquid and vapour products. Consider the bubble point temperature of 97°C and the dew point temperature of 110°C. The vapour pressure vs. temperature data are given in the Figure.



Now, let us consider an example to discuss the flash distillation. A mixture of hydrocarbons containing 32 mole percent of n-hexane, 38 mole percent of n-heptane and 30 mole percent of n-octane is subjected to a flash distillation at 1.2 atmosphere pressure, 40 percent of the feed is to be vaporized.

Find the temperature of the flash and the composition of the liquid and the vapour products. Consider the bubble point temperature of 97 degree Centigrade and the dew point temperature of 110 degree Centigrade. The data the vapour pressure and the temperature data are given in this figure. So, this is the temperature vapour pressure data.

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Example 2: Solution

A mixture of hydrocarbons containing 32 mole% n-hexane, 38 mole% n-heptane and 30 mole% n-octane is subjected to a flash distillation at 1.2 atm pressure and 40% of the feed is vaporized. Find the temperature of the flash and the composition of the liquid and vapour products. Consider the bubble point temperature of 97°C and the dew point temperature of 110°C. The vapour pressure vs. temperature data are given in the Figure.

Solution:

$$\text{Assume } T = 97 + 0.4(110 - 97)$$

$$= 97 + 0.4 \times 13 = 97 + 5.2 = 102.2^\circ\text{C}$$

| | |
|----------------------------------|-------------------------------------|
| $n\text{-}C_6 = 2.5 \text{ atm}$ | $K_{n\text{-}C_6} = 2.5/1.2 = 2.08$ |
| $n\text{-}C_7 = 1.1 \text{ atm}$ | $K_{n\text{-}C_7} = 1.1/1.2 = 0.92$ |
| $n\text{-}C_8 = 0.5 \text{ atm}$ | $K_{n\text{-}C_8} = 0.5/1.2 = 0.42$ |

So, the flash temperature in this case would lie between the bubble point temperature and the dew point temperature. Now, assume T which is flash temperature would be equal to bubble point temperature 97 plus 40 percent is vaporized that is 0.4 into the dew point temperature 110 minus 97 that is the bubble point temperature. So, this would be equal to 97 plus 0.4 into 13 which is equal to 97 plus 5.2 which is 102.2 degree Centigrade.

Now, if we look into the figure this figure at 102 degree Centigrade temperature say over here if you can go up you will obtained for vapour pressure for octane is about 0.5, similarly for n-heptane is about 1.1 and again if you go up over here, so you will obtain is about 2.5. So, from the figure we can write vapour pressure at that temperature is for $n\text{-}C_6$ is about 2.5 atmosphere. Similarly for $n\text{-}C_7$ is about 1.1 and $n\text{-}C_8$ is about 0.5.

Now, we can obtain the K values that is $K_{n\text{-}C_6}$ would be equal to 2.5 divided by the pressure of the operation, that is 1.2 atmosphere. So, which is equal to 2.08, similarly $K_{n\text{-}C_7}$ would be equal to 1.1 divided by 1.2 which is equal to 0.92 and $K_{n\text{-}C_8}$ would be equal to 0.5 divided by 1.2 which is equal to 0.42.

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Example 2: Solution

A mixture of hydrocarbons containing 32 mole% n-hexane, 38 mole% n-heptane and 30 mole% n-octane is subjected to a flash distillation at 1.2 atm pressure and 40% of the feed is vaporized. Find the temperature of the flash and the composition of the liquid and vapour products. Consider the bubble point temperature of 97°C and the dew point temperature of 110°C. The vapour pressure vs. temperature data are given in the Figure.

Solution:

$$\sum x_i = 1.0 = \sum \frac{x_{iF}}{f(K_i - 1) + 1}$$

RHS = $\frac{0.32}{0.4(2.08-1)+1} + \frac{0.38}{0.4(0.92-1)+1} + \frac{0.3}{0.4(0.42-1)+1}$

$$= \frac{0.32}{1.432} + \frac{0.38}{0.968} + \frac{0.3}{0.768}$$

$$= 0.224 + 0.393 + 0.391$$

$$= 1.008, \Rightarrow \text{This is close to unity.}$$

\Rightarrow Flash point temp. $\sim 102.2^\circ\text{C}$

Now we know that summation over x_i is equal to 1.0 which is equal to summation over x_{iF} divided by fraction vaporized f into K_i minus 1 plus 1. Now, if we consider right hand side of the equation we can write 32 mole percent n-hexane, so x_{iF} would be 0.32 divided by 40 percent of the feed is vaporized. So, f would be 0.4 into K_i for component n c 6 as we have calculated K_{nc6} is equal to 2.08 K_{nc7} is equal to 0.92 and K_{nc8} is equal to 0.42.

So, if we substitute this 2.08 minus 1 plus 1, now for the component heptane n c 7 we can write plus which is 38 mole percent. So, 0.38 divided by 0.4 into 0.92 minus 1 plus 1 plus for component n c 8 which is 30 percent so it is 0.3 divided by 0.4 into 0.42 minus 1 plus 1. So, this would be equal to 0.32 divided by 1.432 plus 0.38 divided by 0.968 plus 0.3 divided by 0.768, this would be equal to 0.224 plus 0.393 plus 0.391 which is equal to 1.008. So, this is close to unity.

Hence, flash point temperature is equal to 102.2 degree Centigrade. Now, the liquid composition as we can see from this relation, so this is from here we can get the composition of the n-hexane and this is the composition of n-heptane and this is the composition of n-octane.

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Example 2: Solution

A mixture of hydrocarbons containing 32 mole% n-hexane, 38 mole% n-heptane and 30 mole% n-octane is subjected to a flash distillation at 1.2 atm pressure and 40% of the feed is vaporized. Find the temperature of the flash and the composition of the liquid and vapour products. Consider the bubble point temperature of 97°C and the dew point temperature of 110°C. The vapour pressure vs. temperature data are given in the Figure.

Solution: Liquid composition: n-C₆ = 22.4%
n-C₇ = 39.3%
n-C₈ = 39.1%

The composition of the vapour product is computed from the values of K_i & x_i : $y_i = K_i x_i$

| | | | |
|--------------------------------|---------------------------------|---|--|
| n-hexane (n-C ₆), | $y = 0.224 \times 2.08 = 0.466$ | } | $K_{n-C_6} = 2.08$ $K_{n-C_7} = 0.92$ $K_{n-C_8} = 0.42$ |
| n-heptane (n-C ₇), | $y = 0.393 \times 0.92 = 0.362$ | | |
| n-octane (n-C ₈), | $y = 0.391 \times 0.42 = 0.164$ | | |
| 0.992 | | | |

So, liquid composition n c 6 is equal to 22.4 percent, n c 7 is equal to 39.3 percent, n c 8 is equal to 39.1 percent. Now, the composition of the vapour product is computed from the values of K_i and x_i , as we know y_i is equal to $K_i x_i$. Now, n-hexane n c 5 y vapour composition would be 0.224 into 2.08 which is K_i as we know K_{n-C_6} is 2.08, K_{n-C_7} is 0.92 and K_{n-C_8} is 0.42.

So, this would be equal to 0.46 466, then n-heptane that is n c 7 is equal to 0.393 into 0.92 which is equal to 0.362 and n-octane this would be equal to 0.391 into 0.42 which is equal to 0.164 if we sum up it would be 0.992. So, this is the vapour composition and this is the liquid composition.

So, this way if we have the bubble point and dew point temperature and the composition of the mixture and the pressure of the operations are means and we can calculate the flash point temperature and as well as the liquid and vapour compositions.

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“Key” Components

- Select two components to serve as *heavy key* (H) and the *light key* (L).
- Key components must be present in both the overhead and the bottoms.
- **Light Components:** more volatile than light key are called light components and will be present in bottoms in small amounts.
- **Heavy components:** less volatile than heavy key and present in distillate in small amounts.

Now we need to consider the key component for multicomponent distillation. Select two components to serve as heavy key and the light key. Key component must be present in both the overhead and the bottoms, please remember that key components must be present both in overhead and the bottoms. Then, light components we can define as the more volatile than the light key are called the light components and will be present in bottoms in small amount. Heavy components: less volatile than heavy key and present in distillate in small amount.

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“Key” Components

- Two key components are present in significant amounts in both the distillate and bottoms.
- **Non-key components (everything but the keys):** *distributed* if they occur in both products, or *non-distributed* if they appear in only one product.
- Remember, keys must be distributed.
- Non-keys may be distributed when they have volatilities very close to keys or between keys, and when desired separation is sloppy.

Two key components are present in significant amounts in both distillate and bottoms. So, please note that the two key component should be present in significant amount in both distillate and bottoms. Now, non-key components that is everything, but the keys; that means, it may be distributed if they occur in both products that is bottoms and the distillate or non distributed if they appear in only one product; that means, either in bottoms or in vapour or in distillate they are called non-key components.

Remember, keys must be distributed that is heavy key and light key they must be distributed and they should present in both distillate and bottoms in significant amount. Non-key may be distributed when they have volatilities very close to the keys or between the keys and when desired separation is sloppy.

So, in this lecture we have discussed the introduction to the multicomponent systems and then number of tower requires for a multicomponent systems, different calculation methods, equilibrium in multicomponent systems and bubble point dew point calculations, multicomponent flash distillation and concept of key components and you know minimum number of stages.

So, thank you for attending this lecture and we will continue our discussion on multicomponent system in the next lecture.