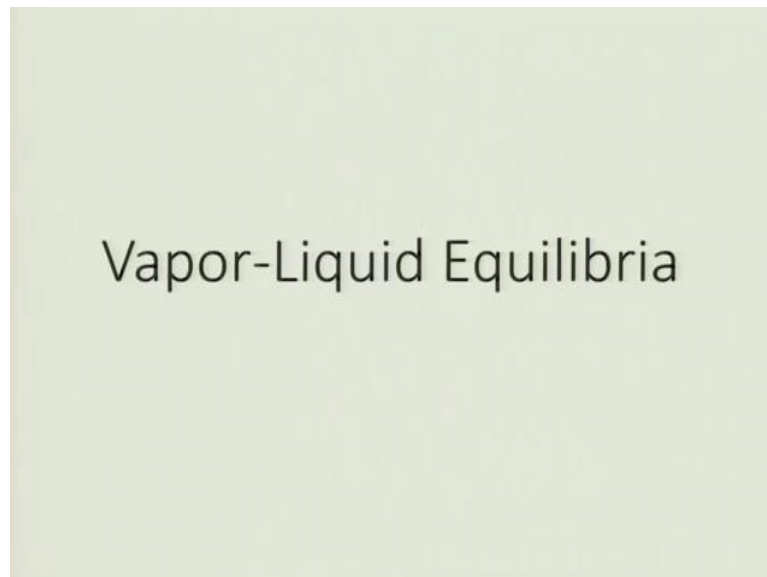


**Chemical Engineering Thermodynamics**  
**Prof. Jayant K. Singh**  
**Department of Chemical Engineering**  
**Indian Institute of Technology Kanpur**  
**Lecture: 49 Vapor-Liquid Equilibria (Examples)**

Welcome back! In the last lecture we talked about methodologies for calculating phase equilibrium particularly the discussion was on vapour liquid equilibrium. So, there we considered the vapor phase in terms of fugacity and the liquid phase in terms of their activity. And then we said well, we will take example of binary mixtures where we consider the ideal gas and vapor phase and basically gas mixtures in the vapor phase and the liquid to be, liquid we consider as an ideal solution.

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### Bubble Point Calculation with P Known

Consider a system with liquid containing 30% *n*-pentane (1), 30% cyclohexane (2), 20% *n*-hexane (3), and 20% *n*-heptane (4) at 1 bar. Determine the temperature at which this liquid develops the first bubble of vapor. What is the vapor composition?

	Bubble Point ( $x_i$ known)	Dew Point ( $y_i$ known)
$T$ known	II Find $y_i, P$ $p_i^{\text{sat}}$ set	I Find $x_i, P$ $p_i^{\text{sat}}$ set
$P$ known	III Find $y_i, T$ $p_i^{\text{sat}}$ unknown	IV Find $x_i, T$ $p_i^{\text{sat}}$ unknown

find  $y_i, T$   
 given  $P$   
 $P, x$

Since the components in this system are chemically similar, we will assume an ideal solution

However we looked at only the binary mixtures and introduce a lecture we are going to extend this understanding and with little bit of more example probably you will be able to grasp this way of finding out the phase diagram or in general we can address the question such as this what we are going to solve now.

So this is on a bubble point calculation with pressure known. And we have discussed about this quadrant. So it is a pressure known bubble point with given pressure, so essentially here the pressure is known so you have to look in this way that find  $y_i$  and  $t$ . So let us, us look at the questions. The question is here on that for a given system with the liquid which contains 30 percent n pentane, 30 percent cyclohexane, 20 percent n hexane and 20 percent n heptane at 1 bar and this 1, 2, 3, 4 this are the basically to indicate this species. So the question is to determine the temperature at which this liquid which contains this 4 component develops the first bubble of vapor and what is the vapor composition? Essential it is talking about  $y_i$ , so find  $y_i$ , temperature is given to you, no the temperature is not given. What is given to you? Given is pressure. So, it is like pressure is known and then find  $y_i$ ,  $t$  which essentially is this quadrant 3.

Here of course if you look at it, we do not have this  $p_i$  set also so that is something which we are going to use. So, considering that the components are similar in nature, the species are the molecules here are similar in nature so essentially, we would be considering ideal solution and a gas phase we can consider ideal gas. So that is approximation we are going to do and we will be calculating the bubble point that means the first the temperature at which the first bubble of vapor form so that is a temperature and as well as we will be finding  $y_i$ .

(Refer Slide Time: 3:09)

## Bubble Point Calculation with P Known

Consider a system with liquid containing 30% *n*-pentane (1), 30% cyclohexane (2), 20% *n*-hexane (3), and 20% *n*-heptane (4) at 1 bar. Determine the temperature at which this liquid develops the first bubble of vapor. What is the vapor composition?

	Bubble Point ( $x_i$ known)	Dew Point ( $y_i$ known)
T known	II Find $y_i, P$ $P_i^{sat}$ set	I Find $x_i, P$ $P_i^{sat}$ set
P known	III Find $y_i, T$ $P_i^{sat}$ unknown	IV Find $x_i, T$ $P_i^{sat}$ unknown

$x_1 = 0.3$  find  $y_i, T$   
 $x_2 = 0.3$  given  $P$   
 $x_3 = 0.2$   $P_i^{sat}$   
 $x_4 = 0.2$

Since the components in this system are chemically similar, we will assume an ideal solution

At 1 bar, we may assume an ideal gas

The criterion for phase equilibrium in terms of Raoult's law for each of the components:

$$y_i P = x_i P_i^{sat}$$

1 bar

$$P = \sum y_i P = \sum x_i P_i^{sat} = x_1 P_1^{sat} + x_2 P_2^{sat} + x_3 P_3^{sat} + x_4 P_4^{sat}$$

Antoine's equation:

$$\ln P_i^{sat} [\text{bar}] = A_i - \frac{B_i}{T[\text{K}] + C_i}$$

NLSF we know

Species	<i>n</i> -C <sub>5</sub> H <sub>12</sub>	C <sub>6</sub> H <sub>12</sub>	<i>n</i> -C <sub>6</sub> H <sub>14</sub>	<i>n</i> -C <sub>7</sub> H <sub>16</sub>
A <sub>i</sub>	9.2131	9.1325	9.2164	9.2535
B <sub>i</sub>	2477.07	2766.63	2697.55	2911.32
C <sub>i</sub>	-39.94	-50.50	-48.78	-56.51

$$y_i P = x_i P_i^{sat}$$

$$P = \sum y_i P = \sum x_i P_i^{sat} = x_1 P_1^{sat} + x_2 P_2^{sat} + x_3 P_3^{sat} + x_4 P_4^{sat}$$

$$\text{Antoine's eqn: } \ln P_i^{sat} [\text{bar}] = A_i - \frac{B_i}{T[\text{K}] + C_i}$$

So, we will start for the same understanding as we have done earlier, we will be considering the Raoult's law to start with and the Raoult's law states that  $y_i p$  which is nothing but the partial pressure is nothing but  $x_i p_i^{sat}$ , so that is our Raoult's law expression. Now  $p$  total pressure is nothing but the sum of the partial pressures  $y_i p$  and that can be written as  $x_i p_i^{sat}$  and now for the 4 component we have to write like this in the 2 component it was straight forward that we

considered  $x_1$  and  $1 - x_1$ , but now there are 4 components and for each of them we have Antoine equation.

So this you can get it from the table so all both you know all the expressions of Antoine equation expression is written in this way where A, B, C these are the constants which one has to extract from the data and usually they are tabulated in the table. So for this problem we have got it from the text book of this course, so this for 4 components we have A, B and C which is known you can also look at NIST we have book that also can give you this, but of course in this case we have the text book which has this data for us.

So basically, it means that for given  $t$  one can find out pressure, but in our case the temperature is not known but of course A, B, C we can get it from this table. So, we can plug in this here and all this expression will be now a function of  $x$  and basically  $t$ . Now sorry, so in this case here the  $y$  is not known, so essentially  $x$  is also given to you. So if you look at it here  $x_1$  is 0.3,  $x_2$  is 0.3 and  $x_3$  is 0.2 and  $x_4$  is 0.2 because this is the liquid composition  $x$  so what we do not know is  $y$  so essentially first the function here is just a function of temperature.

So we plug in here, so this is going to be something like  $x_1$  value is already known and  $p_1^{\text{sat}}$  can be a function of temperature which is let us say  $A - B_1 / t + c_1$  and similarly we can write this and this is going to be  $a_2 - b_2 / t + c_2$ . So  $x_1$  and  $x_2$  we will have so we can use an Excel sheet to find out or you can write this expression and right-hand side of course is 1 bar, so sorry left-hand side is 1 bar. So left hand side is known right hand side  $x$  of course you can plug in what remains is basically a function of  $t$ , which you have to find a  $t$  such that it satisfies left hand equal to right hand side.

(Refer Slide Time: 6:15)

$T=333\text{K}$

iterative calculation  
goal seek solver  
Excel  
R.H.S - 1 = 0  
find t

Species	$n\text{-C}_5\text{H}_{12}$	$\text{C}_6\text{H}_{14}$	$n\text{-C}_8\text{H}_{18}$	$n\text{-C}_7\text{H}_{16}$
$P^{\text{sat}}$ at 333 [K]	2.13 bar	0.514 bar	0.757 bar	0.218 bar
$y_i$	0.639	0.154	0.151	0.056

Note that relatively larger amount of *lighter*  $n$ -pentane goes into the vapor compared to the *heavier*  $n$ -heptane

This result forms the basis for separation by distillation.

At 1 bar, we may assume an ideal gas

The criterion for phase equilibrium in terms of Raoult's law for each of the components:

$y_i P = x_i P_i^{\text{sat}}$   $\Rightarrow y_i = \frac{x_i P_i^{\text{sat}}}{P}$

$1 \text{ bar} = P = \sum y_i P = \sum x_i P_i^{\text{sat}} = x_1 P_1^{\text{sat}} + x_2 P_2^{\text{sat}} + x_3 P_3^{\text{sat}} + x_4 P_4^{\text{sat}}$

Antoine Eq.  $= x_1 \left( A_1 - \frac{B_1}{T + C_1} \right) + x_2 \left( A_2 - \frac{B_2}{T + C_2} \right) + \dots$

Antoine's equation:  $\ln P_i^{\text{sat}} [\text{bar}] = A_i - \frac{B_i}{T[\text{K}] + C_i}$

NLSF  $\ln P_i^{\text{sat}}$

Species	$n\text{-C}_5\text{H}_{12}$	$\text{C}_6\text{H}_{14}$	$n\text{-C}_8\text{H}_{18}$	$n\text{-C}_7\text{H}_{16}$
$A_i$	9.2131	9.1325	9.2164	9.2535
$B_i$	2477.07	2766.63	2697.55	2911.32
$C_i$	-39.94	-50.50	-48.78	-56.51

And if you do this iterations, interactive calculation so you can use again as I said earlier that you can use the goal seek solver of Excel sheet and there you can say that well, the right-hand side function which is of course the function of temperature minus 1 should be 0. So basically, this essentially will become the goal. So, find t in this function such that this whole function or this whole term is basically got it 0 or 1. So you can actually take this also as different way you can consider this to be just 1 that means right hand side is equal to 1. But usually is easier if you just say that function is equal to 0.

That is of the usual way to do that so if you do this exercise the temperature comes out to be this alright. So this is something which you can do in Excel sheet and not showing it but this can be done easily. So for, for the case of this 4 cases, once we have this temperature which we

have evaluated we can find out  $p_{sat}$  we can plugin back this temperature in this expressions and obtain  $p_{sat}$  so that is something which is given here. And now given that  $p_{sat}$  you can now use this because  $x$  we know, so  $y_i$  is nothing but  $x_i$ ,  $p_i$  by  $p$  here. So this we have calculated  $x_i$  we know and pressure is known because that is a one which is given to you.

So from there you can obtain this  $y_i$  so if you look at here the  $y_i$  now calculated and this is the values which we have. So it is a straight forward systematic analysis and the key is that you come up with this expression of the phase equilibrium criteria. In this case we have considered Raoult's law again, why the Raoult's law again? Because of the similar types of the molecules which are non-polar in nature and then subsequently we said well the ideal gas the vapour phase can be ideal gas, liquid phase can be assumed to be ideal gas and then we have this Raoult's law expression and then the condition in that since we know the pressure. Already sub pressure is equal to summation  $y_i p$ . But we do not know the  $y_i$ s.

So that is what we have replace this thing to these expressions based on the Raoult's law and then we have this expression, you replace these parts by this Antoine equation and then you have a function of only temperature. Find out the temperature that satisfy that equation and that is what we got it. And if you note at here note this that the composition this is much, much lower than this and essentially it says heavier this is heptane It is much smaller than that of the pentane.

So the pentane has the highest composition in the vapor phase which is understandable because at a given temperature among the 4 this is the lightest molecule and that is what there will be much, it will be much easier to evaporate the energy required to vapor it from the liquid phase will be less and that is why this is seen, this is also you can find out from the pressure  $p_{sat}$  is much larger here which is also means that the composition in the vapor phase is going to be larger and here the  $p_{sat}$  is lower which also mean the compositions are going to be lower. So it basically it gives you the driving factor as such.

Now because of this nature of this compositional variation based on the temperature among this similar kind of molecule which has different molecular weight, this gives us the basis of separation by distillation where the temperature can be varied by providing the appropriate heat here. So it depends on the clearly, clearly the separation and thus understanding of phase diagram would become a relevant in distillation columns design.

(Refer Slide Time: 10:22)

## Dew Point Calculation with P Known

Consider a system with vapor containing 30% n-pentane (1), 30% cyclohexane (2), 20% n-hexane (3), and 20% n-heptane (4) at 1 bar. Determine the temperature at which this vapor develops the first drop of liquid. What is the liquid composition?

	Bubble Point ( $x_i$ known)	Dew Point ( $y_i$ known)
T known	II Find $y_i, P$ $P_i^{sat}$ set	I Find $x_i, P$ $P_i^{sat}$ set
P known	III Find $y_i, T$ $P_i^{sat}$ unknown	IV Find $x_i, T$ $P_i^{sat}$ unknown

$y_1 = 0.3, y_2 = 0.3, y_3 = 0.3$   
 $y_4 = 0.2$   
at 1 bar  
find  $\{x\}, T$

Write Raoult's law for each species:

$y_i P = x_i P_i^{sat}$   
 $\sum x_i = 1$

$1 = \sum \frac{y_i P}{P_i^{sat}} = \frac{y_1 P}{P_1^{sat}} + \frac{y_2 P}{P_2^{sat}} + \frac{y_3 P}{P_3^{sat}} + \frac{y_4 P}{P_4^{sat}}$

So we can take it forward now we can look at the dew point calculation with p known. So let us first describe the problem and then we can see where they are falling in which coordinate. So here again the we have the similar set for molecules 30 percent n pentane, 30 percent cyclohexane and pentane and 20 percent heptane. However now it is a vapor phase. So this is system with vapor containing this composition that means you have  $y_1$  is 0.3,  $y_2$  is 0.3,  $y_3$  is 0.3,  $y_4$  is 0.2 and this is all at, at 1 bar.

So the question is the t point, finding the t point calculation that means determine the temperature at which this vapor which contains this component at this composition develops the first drop of liquid. That is what the dew is and hence dew point calculation at a given pressure which is 1 bar. So essentially, we need to find, find x and as well as the temperature. So if you look at this the pressure is known but now it is a dew point, so this is what we have to find it out. So given that the temperature is not known, we do not know  $P_i^{sat}$  as o, so  $P_i^{sat}$  is unknown. So we again go back to our Raoult's law because this is a same set of components and hence we are going to use Raoult's law and for each species you have again  $y_i P$  is equal to  $x_i, P_i^{sat}$ . Now what you can do is since you know y so essentially  $x_i$  is not known hence  $x_i$  can be written as in this way.

And since summation of  $x_i$  is 1 so we write it in this way 1 is equal to summation  $y_i P_i^{sat}$ ,  $y_i P$  divided by  $P_i^{sat}$  because  $x_i$  is this  $y_i, P_i^{sat}$ . Now for the 4 components of course we can write it in this way, now  $P_i^{sat}$  we do not know, so need to use Antoine equation. So A, B, C of the coefficients of this Antoine equation we know and we can plug in here with that you have an expression because p we know, p is 1 bar.

$$x_i = \frac{y_i P}{P_i^{sat}}$$

$$1 = \sum \left( \frac{y_i P}{P_i^{sat}} \right) = \frac{y_1 P}{P_1^{sat}} + \frac{y_2 P}{P_2^{sat}} + \frac{y_3 P}{P_3^{sat}} + \frac{y_4 P}{P_4^{sat}}$$

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$\ln P_i^{sat} [\text{bar}] = A_i - \frac{B_i}{T[\text{K}] + C_i}$

Substitution of Equations -with one unknown— $T$ .  
 The temperature can be solved.

$1 = P \left[ \frac{y_1}{P_1^{sat}} + \frac{y_2}{P_2^{sat}} + \dots \right]$   
 $1 = f(T)$   
 $T = 349 [\text{K}]$   
 $x_i P_i^{sat} = y_i P \Rightarrow x_i = \frac{y_i P}{P_i^{sat}}$

**Saturation Pressures and Mole Fractions at  $T = 349 [\text{K}]$**

Species	$n\text{-C}_5\text{H}_{12}$	$\text{C}_6\text{H}_{12}$	$n\text{-C}_6\text{H}_{14}$	$n\text{-C}_7\text{H}_{16}$
$P^{sat}$ at 349 [K]	3.296 bar	0.870 bar	1.256 bar	0.494 bar
$x_i$	0.091	0.345	0.159	0.405

Note that proportionately much more of the heavier  $n$ -heptane is condensed compared to the lighter  $n$ -pentane- helping us separate them by distillation.

So you an expression of the left hand side and the right hand side where left hand side is 1, right hand sides  $y, p$  is here,  $y_i$  is like this  $y_1$  divided by  $p_i^{sat}$ , if you look at it here and then this is  $y_2$  divided by  $p_2^{sat}$  and so forth. So, this we plugin from here now which means that you have function  $y$  is equal to function of  $t$  only. Because rest of the things are known  $p$  we know,  $y$  we know, so only thing is that you know you have to find the temperature such that the left-hand side is such that the right-hand side is 1.

So, this again we can do the same thing we can write down this expression and put this expression in the Excel sheet and use the solver such as a goal seek. So if you do that, if you do this iteratively using the such kind of a module in Excel or you can write a program also which can do that but then you have to guess a temperature and then you have to make use of some kind of algorithm in order to converge this, this expression to 1. And if you make use of let us say goal seek the values comes out to be something like  $t$  is equal to 349.

Now with this temperature known now we can obtain all the calculate  $p_i^{sat}$  which is feasible for all the component that is what it is done here 3.296 for the pentane, hexane, heptane up here hexane and this is a cyclohexane, this is a normal heptane and this is your heptane, cyclohexane,



hexane, normal hexane and this is your normal heptane. So that is we have it so for temperature which we have evaluated you can calculate the  $p_i^{\text{sat}}$  and once you have the  $p_i^{\text{sat}}$  which is this then you can go back and make use of a, make use of this Raoult's law to obtain  $x_i$ . Because we know so  $p_i^{\text{sat}}$  we know so that means I can use  $x_i$  is equal to  $y_i p$  divided by  $p_i^{\text{sat}}$ .

So access to  $x_i$  which you have calculated the values are now can be summarized in this way. So if you look at it you have this  $n$ -pentane which is a lighter one and hence the liquid composition is a lowest among all of this. This is the heaviest and it is a highest composition in liquid phase because it cannot be easily vaporized. Now this composition is very well correlated with a pressure  $p^{\text{sat}}$  also which is an indicator of how easily the molecules can be, molecule can escape from the liquid phase to the vapor phase. Though that truly the fugacity is indicator but this will give you some idea.

So lets have a look at it bit to understand it, so you this 3.296 followed by 1.296, followed by 8.70 and followed by 0.494, so that is a kind of a descending order  $p^{\text{sat}}$  at this particular temperature among all this molecule. This followed by, this followed by, this followed by that. So if you compare, if you look at, if you look at access also it will be lowest followed by this, followed by that and then you have the last. So it is very clear as your  $p^{\text{sat}}$  decreases the composition increases and that is also indicator of that how easily can be correlated. So this helps us also in designing the distillation column, because then you can make use of this, this information.

(Refer Slide Time: 17:15)

### Isotherm Flash VLE Calculation

A compressed liquid feed stream containing an equimolar mixture of  $n$ -pentane and  $n$ -hexane flows into a flash unit as shown in the Figure at flow rate  $F$ . At steady state, 33.3% of the feed stream is vaporized and leaves the drum as a vapor stream with flow rate  $V$ . The rest leaves as liquid with flow rate  $L$ . If the flash temperature is  $20^\circ\text{C}$ , what is the pressure required? What are the composition of the liquid and vapor exit streams?

Mass  
 B: Component a  
 $x_a F = y_a V + x_a L$   
 Assume ideal gas  
 & liq soln  
 $y_a P = x_a P_a^S$

$$x_{a,feed} F = y_a V + x_a L$$

*Assuming ideal gas and liquid soln.  $y_a P = x_a P_a^s$*

So let us now move on and try one interesting problem which is a isothermal flash VLE calculation here we will be using the mass balance as well as the Raoult's law information we want, I mean if you understand this we can take it forward to the distillation column also but let us first try to solve this problem first. So here we have a compressed liquid feed stream which contains an equimolar pentane and hexane, normal pentane which flows into flash unit as shown in figure.

So this is a flash tank you putting this liquid stream so that is liquid and then of course it is at this temperature you are maintaining and then essentially it evaporated some part of it to clear this vapor liquid equilibria. The vapor can be taken out and which has a specific composition  $y_a$  which is pentane and then you have the liquid can be taken out from here which with a composition  $x_a$ . So it separates out with a different composition from the main feed composition which has a specific composition 0.5. So at a steady state 33 percent of the feed stream is vaporized that is what the statement is that 33 percent of this is vaporized to this that means there is relation between the feed value and this vapor here feed. And leaves the drum as a vapor stream with flow rate  $V$ .

The rest leaves as a liquid with a flow rate  $L$ . If the flash temperature is 20 degree celsius what is the pressure required? If the flash temperature is 20 degree celsius what is the pressure required? That means to maintain this (19:5) 20 degree celsius temperature is required and then for that a certain pressure is needed. So if the flash temperature is 20 degree celsius for in order to have this 33 percent till operation of vaporization they have to be certain pressure so that the pressure is necessary, that pressure is normally this pressure which we are talking about the equilibrium pressure. So what is the composition of the liquid and vapor at exit streams. With this  $y_a$  and  $x_a$  we need to find.

So let us start with basic mass balance, so we are going to look at the first component a mass balance. So if you look at component  $a$  so  $F$  is a flow rate so if you multiply that with the  $x_a$  of the feed then this is the amount of the component  $a$  which is given to this kind of a flash drive and this could be shown and as a system. And this must be equal to  $y_a V$  the amount goes to the vapor, vapor stream here exit stream plus  $x_a L$  is the amount which is taken by the liquid exit stream.

So this is a basic component balance for mass, a mass balance for component a. Now as I said that you know they has so this is something like you know your (20:45) but then the flash tank evaporates at this temperature 20 and a liquid phase is at equilibrium. So assuming this as is steady state this is maintain at the equilibrium if you do that an also considering that the molecules are very similar in nature. And hence we can assume to be ideal solution and as well as ideal gas phase here, gas mixture phase. So we can make use of Raoult's law. So assuming, assume ideal gas and liquid solution which means I can write  $y_a p$  is equal to  $x_a p_a^s$ , this something which I can write. So if we can substitute this in here then I can get interesting relation. So if you can substitute here we essentially I can substitute  $y_a$ , so  $y_a$  if I substitute what I am going to get, so let me write it now.

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The image shows handwritten mathematical derivations for component mass balance in a flash tank. The equations are as follows:

$$x_{a,feed} F = \frac{x_a P_a^s}{P} V + x_a L$$

$$= x_a \left( \frac{P_a^s}{P} V + L \right)$$

$$x_a = \frac{x_{a,feed}}{\frac{P_a^s}{P} \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$$

b:

$$x_b = \frac{x_{b,feed}}{\frac{P_b^s}{P} \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$$

$$1 = \frac{x_{a,feed}}{\left( \frac{P_a^s}{P} \right) \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)} + \frac{x_{b,feed}}{\left( \frac{P_b^s}{P} \right) \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$$

$$x_{a,feed} F = \frac{x_a P_a^s}{P} V + x_a L = x_a \left( \frac{P_a^s}{P} v + L \right)$$

$$x_a = \frac{x_{a,feed}}{\frac{P_a^s}{P} \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$$

$$b: x_b = \frac{x_{b,feed}}{\frac{P_b^s}{P} \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$$

$$1 = \frac{x_{a,feed}}{\left( \frac{P_a^s}{P} \right) \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)} + \frac{x_{b,feed}}{\frac{P_b^s}{P} \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$$

So, you have  $x_a$  feed and  $F$  and if you substitute the Raoult's law  $y_a$  from there then I get  $x_a p_a^{\text{sat}}$  by  $p$  multiplied by  $V$  plus  $x_a L$ . So that is going to be  $x_a p_a^{\text{sat}}$  by  $p$ ,  $V$  plus  $L$ . So here  $x_a$  is of course given to us I can obtain  $x_a$  from this rearranging I can get  $x_a$  as  $x_a$  feed divided by  $p_a^{\text{sat}}$  by  $p$ ,  $V$  by  $F$  plus  $L$  by  $F$ . So that is an expression which we can get from this. Now similarly, similar exercise is I can do that for  $b$ . So if I do that  $b$  therefore in the liquid phase then I can obtain  $x_b$  as  $x_b$  feed  $p_b^{\text{sat}}$  by  $p$ ,  $V$  by  $F$  plus  $L$  by  $F$ . So for the liquid phase we have two components so if we add it up of course  $x_a$  and plus  $x_b$  is equal 1 and hence I have now one relation which is simply 1 is equal to  $x_a$  feed divided by  $p_a^{\text{sat}}$  by  $p$ ,  $V$  by  $F$  plus  $L$  by  $F$  plus  $x_b$  feed  $p_b^{\text{sat}}$  by  $p$   $V$  by  $F$  plus  $L$  by  $F$ . Now in order to solve this we need to find the ratio of the  $V$  by  $F$ .

(Refer Slide Time: 24:01)

## Isotherm Flash VLE Calculation

A compressed liquid feed stream containing an equimolar mixture of *n*-pentane and *n*-hexane flows into a flash unit as shown in the Figure at flow rate *F*. At steady state, 33.3% of the feed stream is vaporized and leaves the drum as a vapor stream with flow rate *V*. The rest leaves as liquid with flow rate *L*. If the flash temperature is 20°C, what is the pressure required? What are the composition of the liquid and vapor exit streams?

Handwritten notes on the slide:

$\frac{V}{F} = \frac{1}{3}$   
 $\frac{L}{F} = \frac{2}{3}$

Mass Component a  
 $x_{a,feed} F = y_a V + x_a L$   
 Assume ideal gas & Liq soln  
 $y_a P = x_a P_a^S$

$$x_{a,feed} F = \frac{x_a P_a^S V}{P} + x_a L$$

$$= x_a \left( \frac{P_a^S V}{P} + L \right)$$

$$x_a = \frac{x_{a,feed}}{\frac{P_a^S}{P} \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$$

b:

$$x_b = \frac{x_{b,feed}}{\frac{P_b^S}{P} \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$$

$$1 = \frac{x_{a,feed}}{\left( \frac{P_a^S}{P} \right) \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)} + \frac{x_{b,feed}}{\left( \frac{P_b^S}{P} \right) \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$$

Now the question says that 33 percent of the feed stream is vaporized so essentially *V* by *F* should be 1 by 3 and thus *L* by *F* would be 2 by 3. So that is something which we can do. The other thing is that we need to find out *p<sub>b</sub>* and *p<sub>a</sub>*.

(Refer Slide Time: 24:26)

$P_a^S$  at  $20^\circ\text{C}$  } Antoine Eqn  
 $P_b^S$  at  $20^\circ\text{C}$  }  $A, B, C$

$P_a^S = 0.56 \text{ bar}$   
 $P_b^S = 0.16 \text{ bar}$

Solve for  $P = 0.32 \text{ bar}$

$x_a = 0.40$   
 Results show  $\Rightarrow y_a = 0.70$

## Isotherm Flash VLE Calculation

A compressed liquid feed stream containing an equimolar mixture of n-pentane and n-hexane flows into a flash unit as shown in the Figure at flow rate  $F$ . At steady state, 33.3% of the feed stream is vaporized and leaves the drum as a vapor stream with flow rate  $V$ . The rest leaves as liquid with flow rate  $L$ . If the flash temperature is  $20^\circ\text{C}$ , what is the pressure required? What are the composition of the liquid and vapor exit streams?

$\frac{V}{F} = \frac{1}{3}$   
 $\frac{L}{F} = \frac{2}{3}$

Mass B: Component a  
 $x_{a, \text{feed}} F = y_a V + x_a L$   
 Assume ideal gas & Lig soln  
 $y_a P = x_a P_a^S$

$x_{a, \text{feed}} F = \frac{x_a P_a^S V}{P} + x_a L$   
 $= x_a \left( \frac{P_a^S}{P} V + L \right)$   
 $x_a = \frac{x_{a, \text{feed}}}{\frac{P_a^S}{P} \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$

b:  $x_b = \frac{x_{b, \text{feed}}}{\frac{P_b^S}{P} \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$

$1 = \frac{x_{a, \text{feed}}}{\left( \frac{P_a^S}{P} \right) \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)} + \frac{x_{b, \text{feed}}}{\left( \frac{P_b^S}{P} \right) \left( \frac{V}{F} \right) + \left( \frac{L}{F} \right)}$

Values:  $x_{a, \text{feed}} = 0.5$ ,  $x_{b, \text{feed}} = 0.5$ ,  $\frac{V}{F} = \frac{1}{3}$ ,  $\frac{L}{F} = \frac{2}{3}$ ,  $P_a^S = 0.56$ ,  $P_b^S = 0.16$

So we can obtain  $p_a$  s at 20 degree celcius and  $p_b$  s also at 20 degree celcius through Antoine equation. So where we have to make use of some table again we can make use of the 1 which we have just done or you can use NIST waves so you need to get A, B, C of each both the components if you do that  $p_a$  s is comes out to be 0.56 bar,  $p_b$  s comes out to be 0.16 bar. So this is something which you have to plugin here  $x_a$  b is nothing but 0.5, this 0.5 this is 1 by 3, this is 2 by 3 and this is something which we can clearly get.

So what we have this relation is this something we have just calculated using Antoine equation, so you have an expression which is only where unknown is  $p$ . So this is 0.56, this is 0.16 so if you look at it the unknown is  $p$  and you can solve that equation solving that gives you 0.32 bar. So that is a very simple expression, set of equations which we did and once we have the  $p$  you can easily get the, the composition. Because now you have the composition so you can obtain  $x_a$  from here so  $x_a$  will give you 0.4, once  $x_a$  is known you can use Raoult's law, so Raoult's law of course you can use it here. When  $x_a$  is known,  $p_a$  is known,  $p$  is known so you can get  $y_a$ , So  $y_a$  is.

This is something which what we have done is that we have coupled the basic kind of a unit analysis so here the unit process unit is basically the flash drum and here what we assume that this system is steady and phases which get separated because of the flash or the vaporization they are at equilibrium. Vapor and liquid and then we also assume that the both the phases are ideal gas and liquid solution and from there we use material balance application of Raoult's law and the rest the thing was straight forward because we have to use the Antoine equation to get this saturation pressure and subsequently it was straight forward exercise of making use of all this equations which we have written. We will continue this exercise you know and bring the non-ideality in this analysis and for now that would be the end and we will take it up further in the next class. So see you in next class.