Chemical Engineering Thermodynamics
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Lecture – 32
Phase Equilibrium (VLE) Calculations

Hello and welcome back. In this video, today what we will do is try to look at simple vapor liquid equilibrium calculations. Recall that so far we have looked at a solution thermodynamics, we have looked at excess properties, the type of thermodynamic consistency checks. These excess properties need to satisfy the Gibbs free energy, enthalpy, etcetera, and then the interrelationship between various excess thermodynamic properties.

The idea being we want to understand how a mixture of chemical species behaves in a solution, one of the most commonly used applications of solution thermodynamics is in phase equilibrium calculations. This phase equilibrium calculations serve a variety of purposes in chemical engineering practice including a design of separation processes such as distillation, gas absorption, gas adsorption also of course, etcetera.

So, we will get into more complicated models for VLE calculations in the next video, but in this video, we will look at a very simple calculations based on the concept of Raoult's law.

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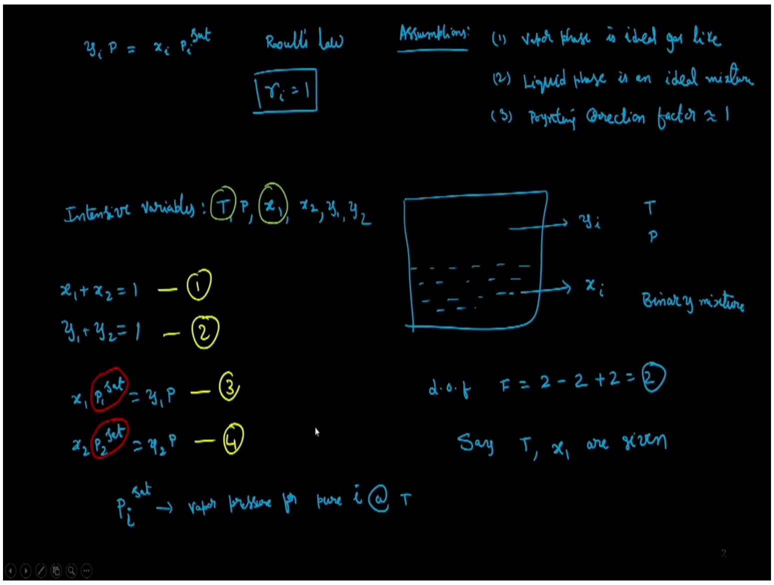

$y_i P = x_i P_i^{sat}$ Raoult's law

$\boxed{\gamma_i = 1}$

Assumptions:
(1) Vapor phase is ideal gas like
(2) Liquid phase is an ideal mixture
(3) Poynting correction factor ≈ 1

Intensive variables: T, P, x_1, x_2, y_1, y_2

$x_1 + x_2 = 1$ — ①
$y_1 + y_2 = 1$ — ②
$x_1 P_1^{sat} = y_1 P$ — ③
$x_2 P_2^{sat} = y_2 P$ — ④

P_i^{sat} → vapor pressure for pure i @ T

d.o.f $F = 2 - 2 + 2 = 2$

Say T, x_1 are given

If you recall, we have developed a model for phase equilibrium in terms of fugacities and then after making the approximation of ideality of the vapour phase, ignoring the pointing correction factor and an ideal mixture in the liquid phase we have come up with the final form of Raoult's law which looks something like this; y i P is x i P i sat. And we call this as Raoult's law, the assumptions were vapor phase is ideal gas like and the liquid phase behaves as an ideal mixture and the pointing correction factor of course is ignored or it is close to 1. And once this happens we can reduce the Raoult's law from equality of the chemical potentials or the fugacities of each of the species.

Now, if you notice there are no activity coefficients in this model which means the activity coefficients for each of the species in this model is 1 that is because we have already assumed the liquid phase to be an ideal solution like. And for an ideal solution, recall that the excess Gibbs free energy is 0 and hence the activity coefficients go to 1. But still it is a good approximation for a variety of mixtures including the ones in homologous series which have similar chemical nature etcetera, one of the famous examples is for a benzene toluene mixture. Now, based on this Raoult's law model for vapour liquid equilibrium we will do some simple calculations in this video, and when we come back in the next video we are going to look at using model for activity coefficient in incorporating that into the vapour liquid equilibrium calculations. But first let us get started with simple calculations.

Let us say I have a binary mixture of a binary mixture, let us say I have a binary mixture in that is at equilibrium in both the vapour and the liquid phases. As usual, we denote the liquid phase composition with the x i, the vapour phase composition with a mole fraction of y i, T is the temperature of this mixture and P is the pressure for this particular mixture.

Now, this is a binary mixture let us say. If I use the phase rule then the degrees of freedom F is going to be the number of components which is two minus the number of phases in this case is 1 vapour, 1 liquid, 2 phases plus 2 which turns out to be 2. So, if I just look at this particular system the intensive variables I am looking at for now are the temperature the pressure and the mole fractions of the liquid and the vapour phases, right. These are the intensive variables I am looking at. And the degrees of freedom is 2 which means I need to fix any two of these variables I have listed here 1 2 3 4 5 6, 6, out of these 6 variables I just need to fix two variables, right and then the other 4 variables are automatically fixed by virtue of the phase rule.

Now, if you recall since this is a binary mixture x 1 plus x 2 is 1, y 1 plus y 2 is 1. So, those are two closure equations which automatically have to hold, right, equation 1 and equation 2 and I am fixing two variables. So, which means now I have 4 equations I still need to write two equations so that I can solve for all the unknowns. The other two equations come from Raoult's law. In this case I can use Raoult's law [noise I can use any phase equilibrium model, but let us say if I use Raoult's law then the other two equations will be x 1 P 1 sat will be equal to y 1 P and x 2 P 2 sat will be equal to y 2 P; now, when I write the other two equations.

So, now, I have 4 equations and 2 degrees of freedom which means I specify two variables. Let us make life simpler. Let us say the temperature and x 1 are given. So, I have temperature and x 1 I am going to circle them in green. These things are given to me and I have 4 equations. So, technically I should be able to find you solve these 4 equations given T and x 1 and I should be able to find the other 4 variables P, x 2, y 1 and y 2. But unfortunately, out of these 4 equations I have two additional variables that show up, one of them is P 1 sat and the other one is P 2 sat. Now, if you recall these are the vapour pressures of pure species 1 and 2 the saturation at the saturation conditions at the equilibrium, right. So, P 1 sat if you recall the way we have derived this phase at the time and we derived this phase equilibrium we said P 1 sat is the vapour pressure for pure 1 at T and or let us just say P i said is vapour pressure for pure species I at the temperature T of interest in this case of that of the mixture.

So, I can solve these 4 equations get the 4 unknowns, but the only catch is that I need to know the vapour pressures for the pure species at the temperature of interest. As long as I have that information, I should be able to solve and get all the other 4 unknowns. Now, let us we are going to solve problems based on binary mixtures because it is easier to handle, but mathematically it should not matter which we should be able to handle, we should be able to solve similar problems even if it is a multi component mixture. Let us extend this discussion to a ternary mixture.

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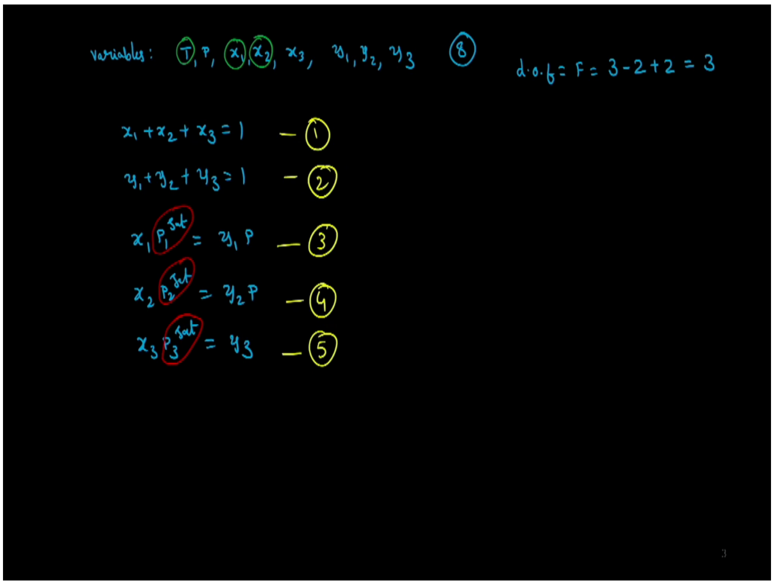

variables : $\textcircled{T}, P, \textcircled{x_1}, \textcircled{x_2}, x_3, y_1, y_2, y_3$ ⑧

$d.o.f = F = 3 - 2 + 2 = 3$

$x_1 + x_2 + x_3 = 1$ — ①

$y_1 + y_2 + y_3 = 1$ — ②

$x_1 P_1^{sat} = y_1 P$ — ③

$x_2 P_2^{sat} = y_2 P$ — ④

$x_3 P_3^{sat} = y_3$ — ⑤

Now, if I have a ternary mixture the intensive variables I am looking at, in this case are the temperature pressure x 1, x 2 and x 3, y 1, y 2 and y 3 the mole fractions in the liquid and the vapour phases.

Now, I have 3 plus 3, 6 plus 2, 8 variables in total. The degrees of freedom for this is the number of components which is 3 minus the number of phases which is 2 plus 2. So, according to the phase rule the degrees of freedom is 3, I need to specify 3 variables to be able to fix the state of the system. So, let us say I fake I choose I can choose any 3 variables, it does not matter. For the sake of discussion, let us choose the temperature x 1 and x 2. If these 3 variables are given then I should be able to find other 5 variables.

Now, to be able to find 5 variables I should write 5 equations. Those 5 equations turn out to be the following x 1 plus x 2 plus x 3 is 1, that is the closure equation for mole fractions in the liquid phase; y 1 plus y 2 plus y 3 is 1 that is the closure equation for mole fractions in the vapour phase that is equation 1 that is equation 2.

So, out of the 8 variables 3 are given I have written two closure equations I need to write 3 more equations and those 3 equations turn out to be the phase equilibrium relations for each of the chemical species. Let us say if I use Raoult's law those fees phase equilibrium relations will be x 1 P 1 sat is y 1 P, x 2 P 2 sat is y 2 P and x 3 P 3 sat will be equal to y 3 P. So, once I have these 5 equations I can solve for the 5 unknown variables.

In this case they are the pressure, x 3, y 1, y 2 and y 3 and then I have my solution for the problem.

Again, the catch being to be able to solve these 5 equations I need knowledge, I need to have knowledge of the 3 vapour pressures P 1 sat, P 2 sat and P 3 sat at the temperature, at the temperature of interest, right. So, if as long as that information is known I can solve the phase equilibrium problem and get the unknown variables. These examples we talked about in case of binary and ternary mixtures are based on picking some variables which are known, but in fact any of these 8 variables in the ternary case can be chosen and the other 5 variables can be solved for using this information.

Since, we said we need to have knowledge of the vapour pressure for the pure species at the temperature of interest where do we get this information from usually we resort to handbooks Perry's handbook is a good example or at the back of your test book for example. There is a list of compounds given and the vapour pressure for these compounds can be calculated using what is known as the Antoine equation.

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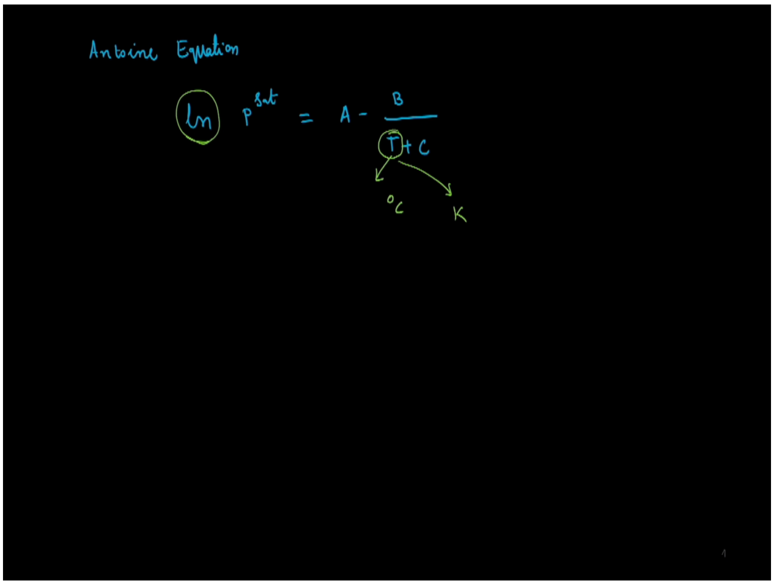

Antoine Equation

$$\ln P^{sat} = A - \frac{B}{T + C}$$

The Antoine equation allows us to calculate the vapour pressure at the temperature of interest the usual form is logarithm of the vapour pressure is equal to A minus B over T plus C. Now, one needs to be careful depending on the source of this information this could be a natural logarithm or log to base 10 for the vapour pressure and the temperature units T need to be specified, right for the particular set of constants we are using.

So, for some source the temperature can be in degree centigrade, for some other source the temperature can be in Kelvin. So, one needs to pay attention to this whether its natural logarithm or the logarithm to base 10, the other thing we need to pay attention when we use this information is what are the units for temperature, is it degree centigrade or Kelvin. As long as we get that information we could use the values of A, B and C from that source and calculate the vapour pressure for pure species. I am sure you heard about Antoine equation earlier we are just revising what you already know, so that we can solve the problems based on this idea.

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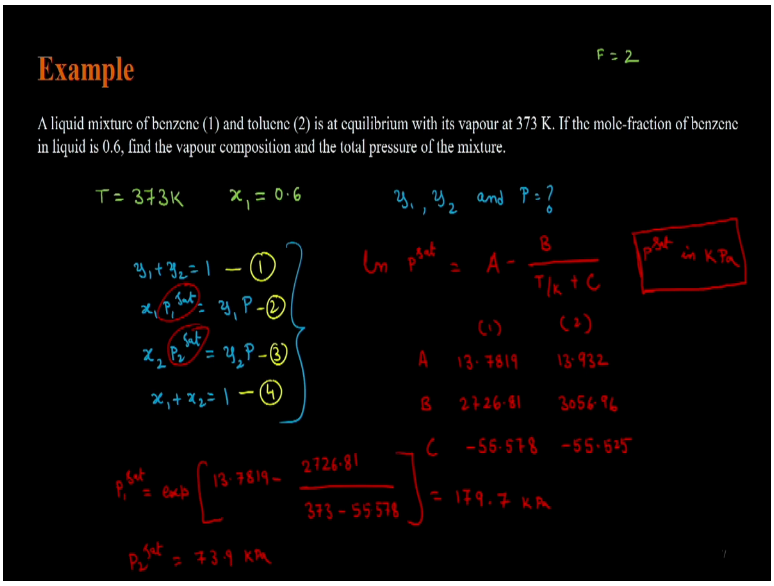

Example

$F = 2$

A liquid mixture of benzene (1) and toluene (2) is at equilibrium with its vapour at 373 K. If the mole-fraction of benzene in liquid is 0.6, find the vapour composition and the total pressure of the mixture.

$T = 373K \quad x_1 = 0.6 \qquad y_1, y_2 \text{ and } P = ?$

$$\left.\begin{aligned} y_1 + y_2 &= 1 \;-① \\ x_1 P_1^{sat} &= y_1 P \;-② \\ x_2 P_2^{sat} &= y_2 P \;-③ \\ x_1 + x_2 &= 1 \;-④ \end{aligned}\right\}$$

$$\ln p^{sat} = A - \frac{B}{T/_K + C} \qquad \boxed{p^{sat} \text{ in KPa}}$$

	(1)	(2)
A	13.7819	13.932
B	2726.81	3056.96
C	-55.578	-55.525

$$P_1^{sat} = \exp\left[13.7819 - \frac{2726.81}{373 - 55.578}\right] = 179.7 \text{ KPa}$$

$$P_2^{sat} = 73.9 \text{ KPa}$$

So, let us get started let us solve a few problems based on a Raoult’s law. The first problem says that we have a liquid mixture of benzene and toluene which is in equilibrium with its vapour at 373 Kelvin. So, the first information that is given to me is that the temperature is 373 Kelvin. This is a binary mixture, so I am going to say that the degrees of freedom is 2. So, there should be two pieces of information that need to be given.

The first one already we know is that the temperature is 373 Kelvin. If the mole fraction of benzene in the liquid is 0.6 so which means in the liquid is x for benzene. We are using a subscript 1, so x 1 is 0.6. Here is our second piece of information. I have T and x

1, once I have T and x 1 we can find the other variables what we want to find in this case is the vapour composition and the total pressure of the mixture.

So, I am interested in knowing what is y 1 and y 2 of course. So, let us write down, that y 1 y 2 and the total pressure of the mixture P, right. That is what I am interested to find. So, there are 3, 3 variables I want to find which means I need to write 3 equations. So, the first equation will be of course, an obvious one y 1 plus y 2 is 1, the second equation is x 1 P 1 sat is going to be equal to y 1 P that is the phase equilibrium relation for component one x 2 P to sat.

The moment I bring in x 2 I am bringing an additional variable whose value I do not know and then there is P 2 sat and P 1 sat, but then we of course, know that x 1 plus x 2 is 1, right. So, I am going to write these 4 equations. And out of these 4 equations I know only the temperature and x 1 in whichever way we can solve. Of course, some of them are obvious ones x 1 is point 1, I can solve equation 4 and say that x 2 is point 4, right. But then it does not matter how you solve these 4 equations as long as we solve them to get all the unknowns we are interested in.

The only catch here is that to be able to you solve all the 4 equations we want still the vapour pressures of the pure species P 1 sat and P 2 sat. Now, to be able to do that, right; to be able to do that we resort to Antoine equations. The Antoine equations am I am going to use will be based on a natural logarithm of P sat at A minus B by the temperature in Kelvin plus C and what I will do is I will list these values of A, B and C for component 1 and component 2 from the source I have used. These numbers turn out to be 13.7819, 2726.81 and negative 55.578 and 13.932, 3056.96, and negative 55.525.

So, this these are the Antoine equations I obtained from a handbook. Once I have these numbers what I can do is in fact these Antoine equations will give me P sat in kilopascals by the way. So, the constants we use will be based on a particular set of units for the vapour pressure for the temperature and whether it is a natural logarithm or logarithm to base 10 etcetera.

Now, in this case I can get p1sat will be exponential of 13.7819 minus B is 2726.81 over temperature is 373 Kelvin minus C is 55.578, and once I solve this what I get for P 1 saturation pressure for one is 179.7 kilopascals. And similarly, I can use the other set of parameters to get P 2 sat to be 73.9 kilopascals.

Now, notice that the at the same temperature of 373 Kelvin the pure component vapor pressure for benzene is higher, so we call it as more volatile and the vapour pressure for toluene is lower so, it is the less volatile component, right. Once I have P 1 sat and P 2 sat from the Antoine equation I can go back and solve all the 4 unknowns.

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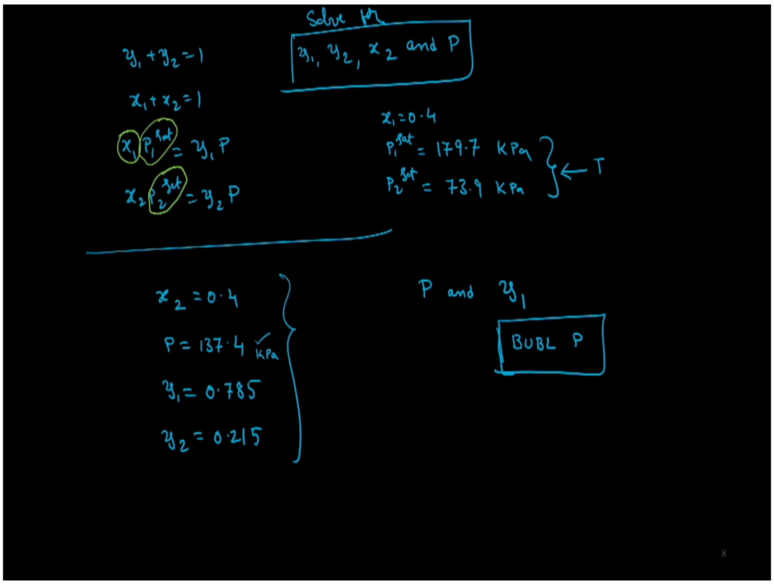

Solve for

$\boxed{y_1, y_2, x_2 \text{ and } P}$

$y_1 + y_2 = 1$

$x_1 + x_2 = 1$

$x_1 P_1^{sat} = y_1 P$

$x_2 P_2^{sat} = y_2 P$

$x_1 = 0.4$

$\left.\begin{array}{l} P_1^{sat} = 179.7 \text{ KPa} \\ P_2^{sat} = 73.9 \text{ KPa} \end{array}\right\} \leftarrow T$

$\left.\begin{array}{l} x_2 = 0.4 \\ P = 137.4 \text{ KPa} \\ y_1 = 0.785 \\ y_2 = 0.215 \end{array}\right\}$

P and y_1

$\boxed{\text{BUBL P}}$

I want to in this case let us rewrite the equations we have y 1 plus y 2 is 1, x 1 plus x 2 is 1, x 1 P 1 sat is y 1 P, x 2 P 2 sat is y 2 P. What I know from after I calculated the Antoine constant from the Antoine equations, I know P 1 sat P 2 sat and x 1, right. Once I have these 3 variables I can use the 4 equations and calculate the 4 unknowns, in this case they are y 1 y 2 x 2 and P. You can solve these 4 equations 1, 2, 3 and 4 for these 4 variables and then we have our result.

You can use any suitable software some of these equations you might be able to solve them by hand, otherwise any suitable software will just do fine. In this case once I do that exercise recall that x 1 is 0.4, P 1 sat we said is 179.7 kilopascals based on Antoine's equation, P 2 sat is 73.9 kilopascals from Antoine's equation. So, this is where we are using temperature information. Based on the temperature information we get P 1 sat and P 2 sat, x 1 of course, we are going to use the in these set of equations, we solve these 4 equations for the 4 unknowns and the final solution I have of course, is an obvious one x 2 is 0.4, then I have a total pressure of 137.4, y 1 I get is 0.785 and y 2 is 0.215. Of course, these two again add up to one. So, these are the 4 variables I get by solving these 4 equations.

So, if we are asked to find the total pressure in this case the total pressure turns out to be 137.4 kilopascals and the mole fraction of the vapour turns out to be 0.785 for benzene and 0.215 for toluene. Remember, we have solved for P and y 1, y 1 is the vapour phase composition and P is the total pressure we call such a calculation as a bubble P calculation. Bubble representing the vapour bubble a mole fraction of the vapor bubble and then P representing the total pressure. So, we call such a calculation where we are solving for y 1 and P as a bubble P calculation.

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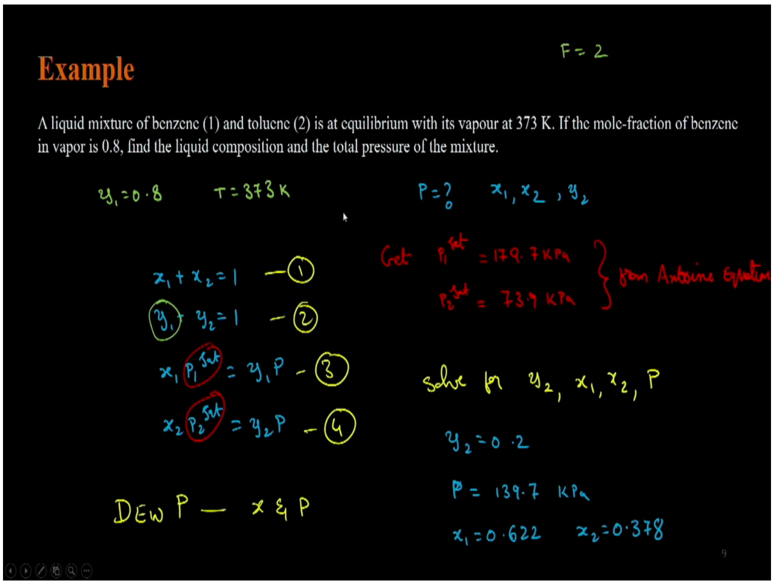

Example

$F = 2$

A liquid mixture of benzene (1) and toluene (2) is at equilibrium with its vapour at 373 K. If the mole-fraction of benzene in vapor is 0.8, find the liquid composition and the total pressure of the mixture.

$y_1 = 0.8$ $T = 373\,K$ $P = ?$ x_1, x_2, y_2

Get $P_1^{sat} = 179.7$ KPa, $P_2^{sat} = 73.9$ KPa } from Antoine Equation

$x_1 + x_2 = 1$ — ①

$y_1 + y_2 = 1$ — ②

$x_1 P_1^{sat} = y_1 P$ — ③

$x_2 P_2^{sat} = y_2 P$ — ④

solve for y_2, x_1, x_2, P

$y_2 = 0.2$

$P = 139.7$ KPa

$x_1 = 0.622$ $x_2 = 0.378$

DEW P — x & P

Let us solve another example. In this case we again have benzene and toluene at 373 Kelvin, but what we are given is that the mole fraction of benzene in the vapour is 0.8.

So, what I have is y 1 equals 0.8; the temperature is still 373 Kelvin. I have the two pieces of information I need recall this is a binary system, so the degrees of freedom is 2. I have the two pieces of information I need what I want to find is the liquid composition and the total pressure of the mixture. So, we want to find P and x 1, x 1, x 2, and of course, y 2.

So, to be able to solve for these 4 variables we write the two closure equations which read x 1 plus x 2 is 1, y 1 plus y 2 is 1 and then the two phase equilibrium relations which will read x 1 P 1 sat is y 1 P, x 2 P 2 sat is y 2 P. Notice that nothing has changed from the previous strategy. These are the same set of 4 equations we are writing. The only thing that is different is that in this case what I know is different I know y 1 and I know the temperature which in turn will give me via the Antoine equations it will give me P 1 sat and P 2 sat.

At 373 Kelvin, I will use the Antoine constants from the previous problem right. And at 373 Kelvin the temperature is still the same. So, I can use the same strategy to calculate P 1 sat and P 2 sat since the temperature is same the pure component of vapour pressure are still going to be the same 179.7 Kelvin sorry kilopascal and 73.9 kilo Pascal. So, let us use those two numbers again. 179.7 kilopascal and P 2 sat is 73.9 kilopascal from Antoine equation, right.

Once I get these two, then I can solve these 4 equations for the 4 unknowns, 1, 2, 3 and 4 equations for the 4 unknowns which happened to be y 2, x 1, x 2, and P. And once we do that the final result I get happens to be of course, y 2 is 0.2 that is trivial. The total pressure in this case turns out to be 139.7 kilopascals and x 1 I get is 0.622, the mole fraction in the liquid phase and x 2 is 0.378, right.

So, I can solve for the 4 unknowns using these same set of 4 equations it is just what the information I have is different, but then the same equations can be used to get what I need. So, since in this case we are we are calculating for x and P, we call such a calculation as a DEW point or the x representing the liquid droplet composition and the pressure is P. So, we call such a calculation as a DEW P calculation, right.

So, notice that the set of equations we are using has not changed, depending on what information I have we just rework the strategy and calculate the unknowns.

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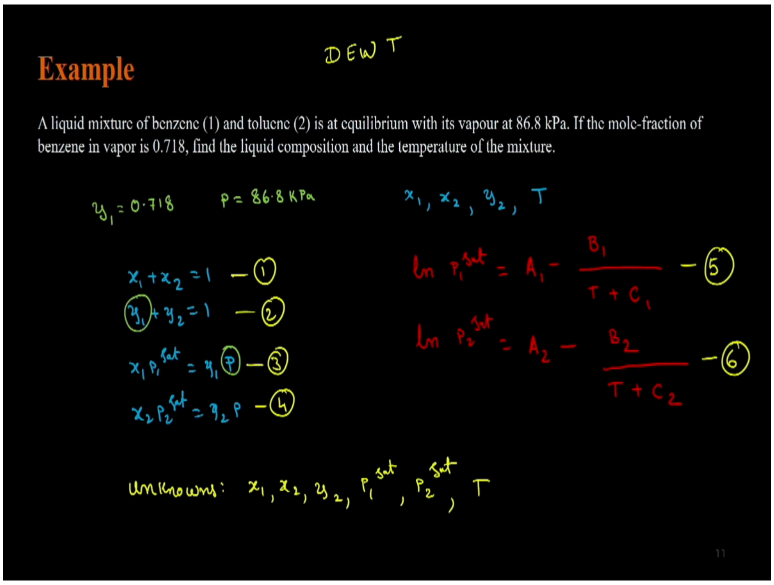

Example

DEW T

A liquid mixture of benzene (1) and toluene (2) is at equilibrium with its vapour at 86.8 kPa. If the mole-fraction of benzene in vapor is 0.718, find the liquid composition and the temperature of the mixture.

$y_1 = 0.718$ $P = 86.8$ KPa

x_1, x_2, y_2, T

$x_1 + x_2 = 1$ — ①

$y_1 + y_2 = 1$ — ②

$x_1 P_1^{sat} = y_1 P$ — ③

$x_2 P_2^{sat} = y_2 P$ — ④

$\ln P_1^{sat} = A_1 - \dfrac{B_1}{T + C_1}$ — ⑤

$\ln P_2^{sat} = A_2 - \dfrac{B_2}{T + C_2}$ — ⑥

Unknowns: $x_1, x_2, y_2, P_1^{sat}, P_2^{sat}, T$

Let us try to solve another problem. In both the previous problems what is given to us is the temperature. Now, in this problem we are given the vapour phase mole fraction and the total pressure and we want to find the temperature and the liquid composition, right. So, what is given to us is the vapour mole fraction y 1 is 0.718 and the total pressure as 86.8 kilopascals.

What I want to find is x 1, x 2, of course, an outcome of that will be y 2 in addition to y 1 and the temperature T, I want to find these 4 variables. So, first thing I would do is write this set of equations I want to solve. The two closure equations which read x 1 plus x 2 is 1, y 1 plus y 2 is 1, those are the two equations I have 1, 2. The two phase equilibrium relations which read x 1 P 1 sat is y 1 P and x 2 P 2 sat is y 2 P. Those are another two equations that make it to a total of 4. Ideally this would have been enough, but then unfortunately I have introduced two additional variables we have equations 3 and 4, those are P 1 sat and P 2 sat.

Now, in the previous two problems because the temperature is given, we said I am going to go to a handbook calculate P 1 sat and P 2 sat at the temperature of interest come back and solve these 4 equations for the 4 unknowns. But now I do not have that luxury, I do not have the temperature, so I cannot calculate the vapour pressures P 1 sat and P 2 sat directly. Temperature also needs to be calculated. So, the way we solve this is bring in the additional two equations, one those happen to be the Antoine relations, one for component one which reads ln of P 1 sat. I do not know P 1 sat what that number is going to be neither I know the temperature, but I know the relation between them it turns out to be A 1 minus A 1 T 1 plus C sorry, T plus C 1 and logarithm of P 2 sat happens to be A 2 minus B 2 by T plus C 2.

I am going to go back to my handbook get the values of A 1, B 1 and C 1 and then write the equation that relates P 1 sat to the temperature which happens to be equation 5 here and P 2 sat to temperature which happens to be equation 6 here. Now, I have 6 equations. I only know two variables y 1 and P, right. Let us highlight the things I know. I only know y 1 and P. I do not know anything else in these 6 equations, but let us count how many variables are unknown. If I write the unknown variables oh let us write in yellow so that we match them with the number of equations unknowns.

In this case are x 1, x 2, y 2, P 1 sat, P 2 sat, that happened to be in the first 4 equations and if you look at 5 and 6, in fact P 1 sat and P 2 sat are already covered, but there is a T which is also unknown. So, I have 1 2 3 4 5 and 6 unknown variables and I have 6 equations that can be used to solve for these 6 unknown variables. It takes a lot of effort to get to the solution manually. So, you could use a convenient software be it MATLAB or if you are good at excel you can set up your equations and use a solver to solve for the unknowns, but whichever way you do it once you solve these 6 equations to get the 6 unknowns you will have your result.

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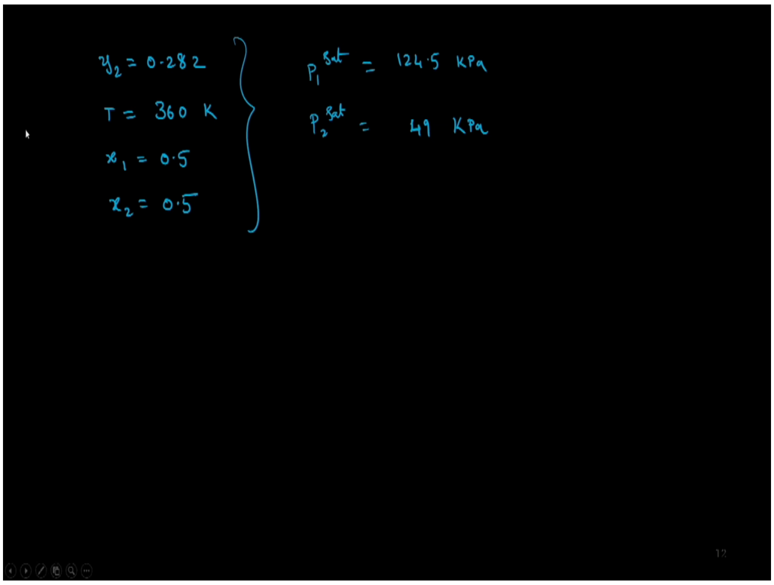

$y_2 = 0.282$

$T = 360 \text{ K}$

$x_1 = 0.5$

$x_2 = 0.5$

$P_1^{sat} = 124.5 \text{ KPa}$

$P_2^{sat} = 49 \text{ KPa}$

In this case I have done that exercise and what I end up with is the obvious value which is for y 2 which is 1 minus y 1 is 0.282 right and then the pressure is given, but the temperature is not the temperature I get is 360 Kelvin, x 1 I have is 0.5 which also makes the value for x 2 to be 0.5, right. These are the 4 variables. This is what I am interested in, but on the side I also end up when I solve the 6 equations I end up getting these two variables P 1 sat happens to be 124.5 kilopascals and P 2 sat happens to be 49 kilopascals at this temperature, right So, these are the 6 variables I end up getting when I solve these 6 equations, right x 1, x 2, y 2 the temperature P 1 sat and P 2 sat, x 1, x 2, y 2 the temperature P 1 sat and P 2 sat.

So, still the same set of equations, the 4 equations, but then because I do not know the temperature essentially I am adding these two as equations instead of plugging in the values of P 1 sat and P 2 sat in these 4 equations. And once you solve these 6 equations together we have the solution to our problem. In this case again we are finding the liquid composition, right. So, it is a DEW and the temperature T. So, it is a DEW T calculation is what it is called, right.

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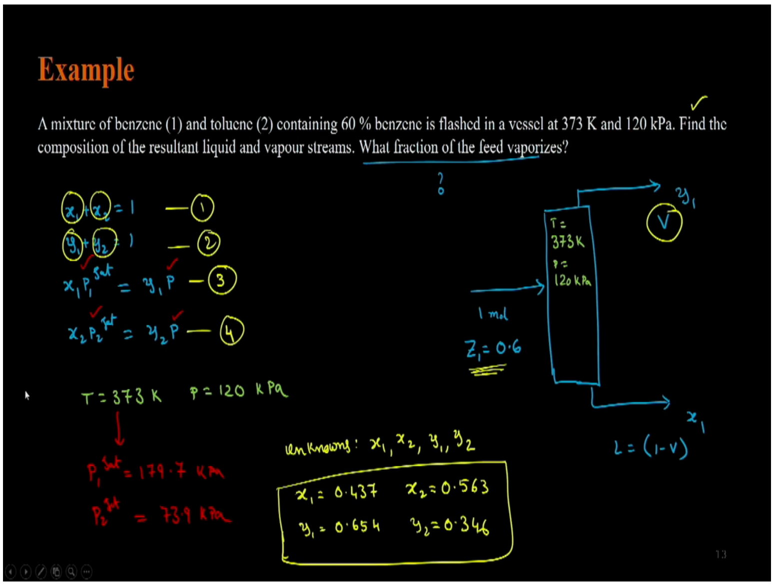

Example

A mixture of benzene (1) and toluene (2) containing 60 % benzene is flashed in a vessel at 373 K and 120 kPa. Find the composition of the resultant liquid and vapour streams. What fraction of the feed vaporizes?

$x_1 + x_2 = 1$ — ①

$y_1 + y_2 = 1$ — ②

$x_1 P_1^{sat} = y_1 P$ — ③

$x_2 P_2^{sat} = y_2 P$ — ④

$T = 373\ K \quad P = 120\ kPa$

$P_1^{sat} = 179.7\ kPa$

$P_2^{sat} = 73.9\ kPa$

unknowns: x_1, x_2, y_1, y_2

$$\boxed{\begin{array}{ll} x_1 = 0.437 & x_2 = 0.563 \\ y_1 = 0.654 & y_2 = 0.346 \end{array}}$$

Now, here is another type of calculation. Now, here is another type of calculation. What we are given is that a mixture of benzene and toluene is flashed into a vessel. This vessel is at 373 Kelvin, well that is a given information, right, so let me use my colour code. The temperature is 373 Kelvin in green and the pressure is 120 kilopascals and also in green. So, this is the pressure, this is the temperature that is given to us. This mixture is flashed in a drum and when we do that we end up with two streams, a liquid stream and a vapour stream.

The mole fraction of the vapour stream is y 1 the mole fraction of the liquid stream is x 1 for benzene, of course and what we are interested in is the compositions y 1 and x 1 and in addition to that we also want to know what fraction of the feed vaporizes. So, for every one mole of feed going in if V moles vaporize then 1 minus V moles will be in the liquid phase. So, we are interested we can call it as L or 1 minus v. So, we are interested in finding this fraction V for every mole of feed that goes in. So, this is our problem.

Now, if you want to solve this problem our approach is still going to be same with a slightly our approach is still going to be the same we are going to use the Raoult's law for phase equilibrium definition. We will write all the set of equations we know. In addition to what we have already used the only difference here is that the feed containing 60 percent benzene it is a mixture it can be a mixture of a liquid and vapor as feed or it can be only depending on the conditions of the feed. We do not know what conditions temperature and pressure conditions it is coming at. It can be only liquid, only vapour or a mixture of liquid and vapour whatever it is. The composition of benzene in this feed is 60 percent. So, what we usually do is use a variable Z in this case for benzene it is subscript of 1, Z 1 is 0.6. This is the overall mole fraction of benzene in the feed depending on what phase it is in it does not matter, but that is the overall composition is what we call it.

Now, we are given two variables in addition to the overall composition. For this particular problem I can still write the same set of equations as earlier, x 1 plus x 2 still needs to be equal to 1, y 1 plus y 2 still needs to be equal to 1, the Raoult's law needs to be satisfied for phase equilibrium, x 1 P 1 sat is y 1 P, x 2 P 2 sat is y 2 P, right. I know the temperature and the pressure, right. Once I know the temperature I can use Antoine equation to get P 1 sat and recall that for benzene and toluene mixture you based on the Antoine constants we had, P 1 sat is 179.7 kilopascals and P 2 sat is 73.9 kilopascals. So, I know the temperature the pressure P 1 sat and P 2 sat. I can solve the equations above to get the 4 unknowns. Oh, I am sorry 2, 3 and 4.

These 4 equations I know P 1 sat. Let us check what we know we know P 2 sat, we know the pressures. So, in these 4 equations the only unknowns are x 1, y 1, x 2 and y 2. I can solve these 4 equations to get the 4 unknowns these 4 unknowns and we have a part of our solution. Once I do this exercise what I get is x 1 happens to be 0.437, x 2 happens to be 0.563 and y 1 happens to be 0.654 and y 2 happens to be 0.346.

So, I got my 4 variables I am interested in by solving these 4 equations. So, I got the first part of this problem by just solving whatever equations we worked with earlier, the Raoult's law equations and the closure equations to get the 4 unknowns. Given the temperature and pressure I found in this case x 1, x 2, y 1 and y 2 by solving these 4 equations that is pretty straightforward.

The second part of the problem says what fraction of the feed vaporizes or I am interested in calculating this quantity V and recall that I still did not use this information the overall mole fraction z 1 is 0.6.

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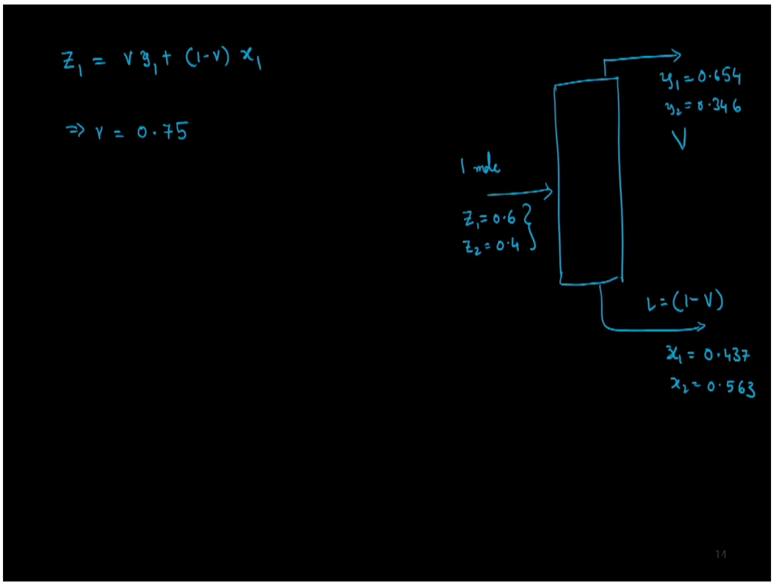

Now, let us see how we do that. I am going to draw that figure again here. Oh, this is y 1, y 1 and this time we solve for y 1 it happens to be 0.64 and y 2 is 0.346. I do not know what that fraction b is, x 1 we solve for it is 0.437 and x 2 is 0.563 and this fraction is 1 minus we can call it as L or it has to be 1 minus V for every mole going in. The overall mole fraction z 1 is 0.6 and z 2 is 0.4, done. So, this is what I have. The temperature and pressure of course, are given.

But now, if you look at this problem and if you are all you are interested is in finding V by the looks of it is a straight math straightforward mass balance problem, 1 mole going in V moles coming out as vapour 1 minus V moles coming out as liquid. So, if I do a component balance then z 1 should be equal to V times y 1 plus one minus V times x 1. I know z, x 1 and y 1 I can solve this equation to find v, right, I can solve this equation to find V and that fraction V in this case turns out to be 0.75, 0.75. So, it means 75 percent of the feed will appear in the vapour phase and 25 percent will appear in the liquid phase.

In addition to this calculation there is one important criteria, when a mixture can be flashed and you will get a split between the vapour and liquid phases, we did not look at that. But usually when we solve this problem a good approach is to actually calculate a dew point pressure and a bubble point pressure, right. We are given the temperature. So, before we do that let us just say that we completed solving this problem. All we did to solve this problem is solve the same set of 4 equations with the different known values and calculated the other unknowns here, in this case the xs and ys. Once we do that we can go back and do a simple mass balance calculation to get the vapour fraction out of this flash tower.

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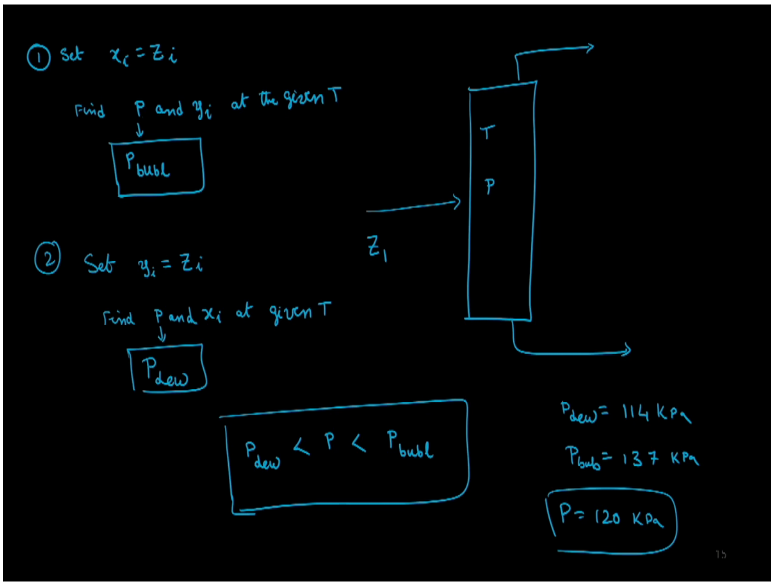

The other thing we were talking about when whenever a flash operation is done, right it is done at a particular temperature and particular pressure with a mole fraction of z 1. So, when we when we have such a scenario where I am given the overall mole fraction and the temperature and pressure of the flash tower the first thing we usually do is set x i the liquid mole fraction to be same as z i, right the given feed composition and find P and y i at the given T, right. So, the temperature is given x i's are given I can find P and y i and we call such a P as a calculation resulting from the bubble P calculation, right. So, we let us call it as P bubble.

The second thing we do is set this vapour mole fraction to be same as z i and then find P and x i at the given T, and since we are doing a P and x i calculation it is a dew T calculation. So, the P, resultant P is what we call as P dew, right this resultant P is what we call as bubble this is P dew.

Now, for a flash operation to be viable and to make sure that we get a liquid and a vapour fraction it turns out that the P dew should be less than P, should be less than P bubble if the pressure at which we are operating the flash tower is not between the dew point and the bubble point pressures then we will not have a flash operation. In the previous example it turns out that the P dew was about a 114 kilopascals and P bubble was about a 134 kilopascals or 137 kilopascals and our P was 120. So, it because it is between the dew point and the bubble point pressures flash operation was viable and we got a solution to our problem. If it was not then we would not have any solution to our problem.

So, this is something to pay attention to whenever we are solving a flash problem the first thing we probably should do is actually calculate the dew point and the bubble point pressures. Make sure that the operation of the flash tower is occurring in between these pressures and then go and solve for the variables we are interested in as we have done in this case, right.

So, that summarizes various types of calculation we can do using Raoult's law. Now, when we come back in the next video, we will look at extending this discussion for non ideal solutions for those mixtures where activity coefficient is not unity.

Thank you.