Aspen Plus Simulation Software – A Basic Course For Beginners

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Lecture-19
Miscellaneous Practice Problems and Case Studies

Welcome to the massive open online course on aspen plus.

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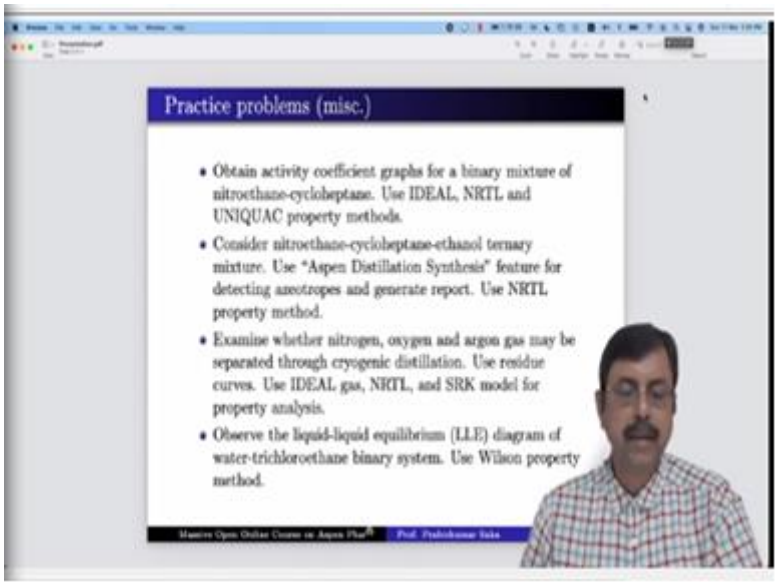

In today's lecture, I shall discuss some practice problems, which are miscellaneous, unlike the last two lectures when we discussed the binary mixture or pure components. In this lecture, we shall talk about some miscellaneous problems, four in numbers.

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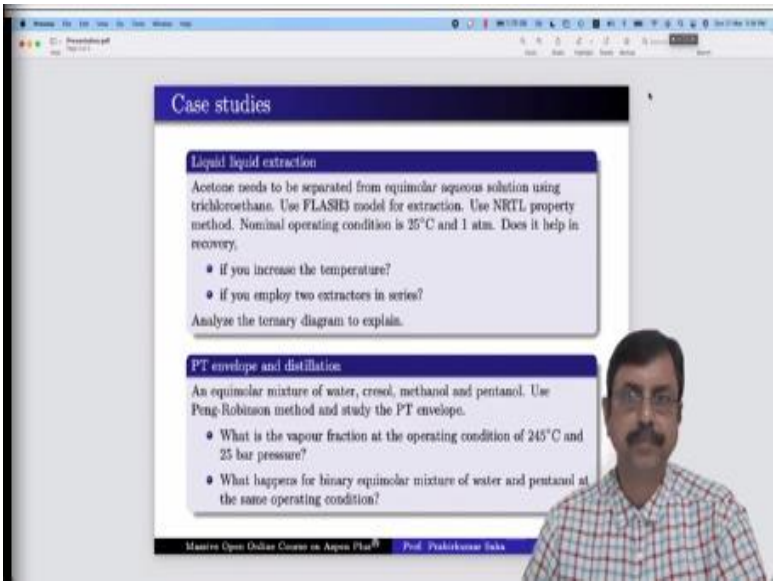

Then, we shall perform two case studies in detail.

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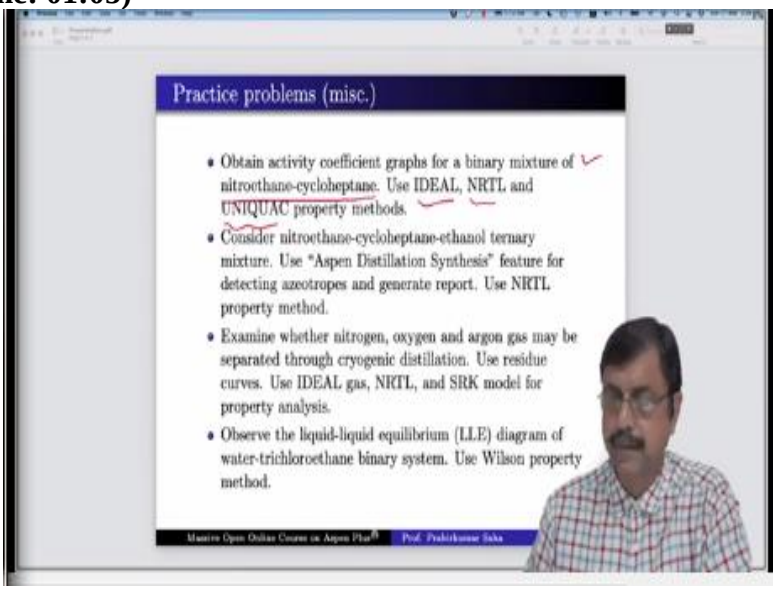

The first practice problem that we will do is about obtaining the activity coefficient graphs for binary mixture of nitroethane and cycloheptane. And we shall use IDEAL method, NRTL method and UNIQUAC property method and analyze the situation. Whatever happens by using these methods we will see and analyze? Let us go to the aspen simulation window. **(Video Starts: 01:40)**

So, here we have to add the components. The first component is nitroethane, so we have to find nitroethane. This is the one we add it. And the second component is cycloheptane, this is the one. So, we rename it NITROETH and CYCLOHEP, now press, Next. So, we shall use 3 property methods IDEAL, NRTL and UNIQUAC. So, first one is IDEAL, then NRTL and UNIQUAC, so the three methods we run.

Now we have to look for the activity coefficient graph of the binary mixture. So, let us bring in the binaries tool, here we have to begin with T-xy. First let us choose IDEAL and then run analysis. We have assumed it is an IDEAL system. So, the graph looks like that of an IDEAL system. So, anyway, we are not interested in the T-xy plot. We have to look for the activity coefficient plot.

As we know, the activity coefficient of an IDEAL system is always 1, so we expect that we will get a curve of unity, which is what we get here. So, the value of the activity coefficient is 1 at any mole fraction of nitroethane or cycloheptane. Next, we shall take the NRTL property method in the calculation option. So, just press NRTL and redo the binary analysis, again we obtain the T- xy plot and this is strange it looks like it is as good as an IDEAL plot.

So, anyway, let us see what the activity coefficient looks like and yes, the activity coefficient again is saying it is 1. So, even the NRTL system suggests that the activity coefficient is 1, which means it is identical to an IDEAL condition. But it is strange NRTL should not give this kind of result. Let us see what unique work property method suggests. So, let us take unique work and redo the binary analysis.

Here we get slight difference from the IDEAL system or for that matter NRTL system. Now let us check the activity coefficient curve, yeah now we are getting some different nature obviously, it is not much the activity coefficient is coming down from 1 to 0.943. So, the difference is not much, so the scale of the y-axis is very narrow. As if the activity coefficient does not change with the mole fraction of nitroethane.

Anyway, at least we are getting some change from ideality, but we are concerned why the NRTL method does not change activity coefficient. For that, let us go back to our NRTL method and check their parameters. The binary parameters of NRTL method and here we find the binary parameters of NRTL method and we are surprised to know that none of the binary parameters have been calculated Aij, Aji, Bij, Bji through Eij and Fij, Fji nothing has been calculated.

That is the reason it is showing the result as good as the IDEAL method, it does not mean that NRTL method is equivalent to IDEAL method. So, what we shall do? We shall take this

estimate using UNIFAC. So, the moment we do it and run, all the missing parameters at least the maximum parameters of NRTL are being computed through UNIFAC. Now we go back to our binary input, calculation option NRTL and see the analysis once again.

And yes, now the T-xy diagram is different from the IDEAL property diagram, which means NRTL has calculated it properly. Anyway, let us not bother about the T-xy diagram. We go to the activity coefficient diagram and find activity coefficients changing with mole fraction of nitroethane, which is expected. For the NRTL property method, this kind of graph is expected, so it decreases from 8 to 1 and liquid cycloheptane. The activity coefficient increases from 1 to 4.6 with increase in the mole fraction of nitroethane. And this result corresponds to 1 atm pressure. If we increase the pressure, this figure will also change. **(Video Ends: 10:16)**

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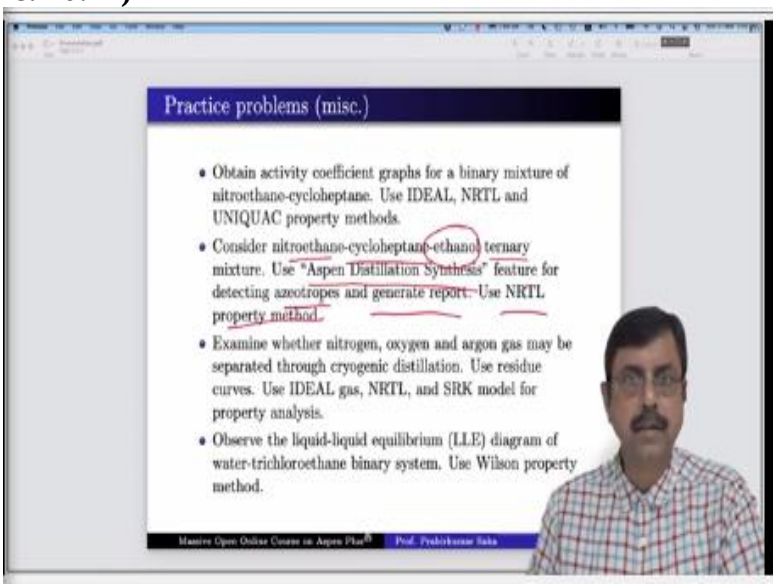

Now let us go to the second practice problem that we have, it is about considering the ternary mixture. So, we add the 3rd component with the system that we just talked about, that is nitroethane and cycloheptane, we add the 3rd component that is ethanol. So, it becomes ternary mixture. Now we have to use aspen distillation synthesis feature for detecting azeotropes and we have to generate a report and here we will use the NRTL property method. So, for that let us go back to the aspen simulation window once again. **(Video Starts: 11:03)**

So, add those components nitroethane, add it, then cycloheptane, add it, and finally, take ethanol. So, just rename it, press next, take NRTL method, run, ok so this time we will not make that mistake, go to the binary parameters, choose NRTL and say estimate using UNIFAC

and we will run it once again. So, it has run, it has estimated all missing parameters with UNIFAC.

Now we shall go to the ternary diagram, so let us bring the ternary diagram tool, here a dialog box appears. The dialog box is distillation synthesis. So, precisely that is what we are asked to do use the "Aspen Distillation Synthesis" feature for detecting azeotropes and generating report. So, every time you press the ternary diagram button, this dialogue box appears.

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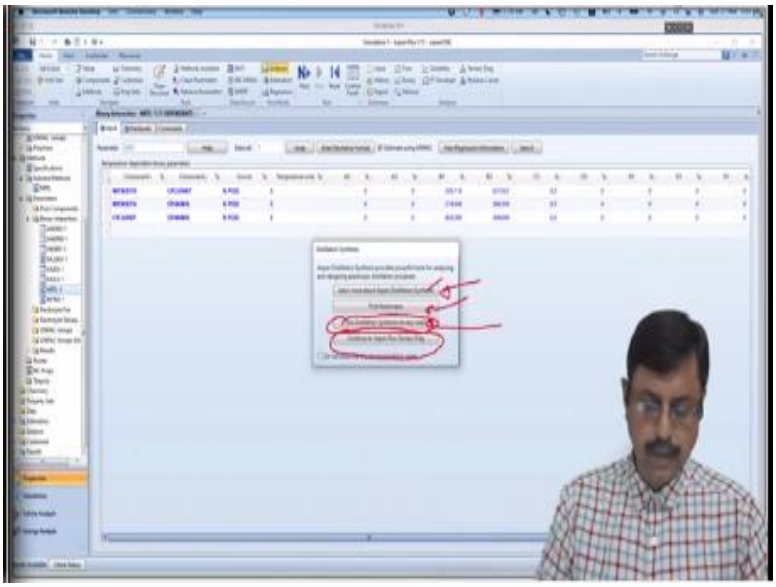

Usually, we choose this particular button because we continue to do the Aspen plus ternary diagram, but it also has other features. You can learn more about Aspen distillation synthesis by pressing this button or you can find the azeotropes by pressing this button. And you can use distillation synthesis ternary map by pressing this button. In this exercise, we will use this 3rd button that is use distillation synthesis ternary maps.

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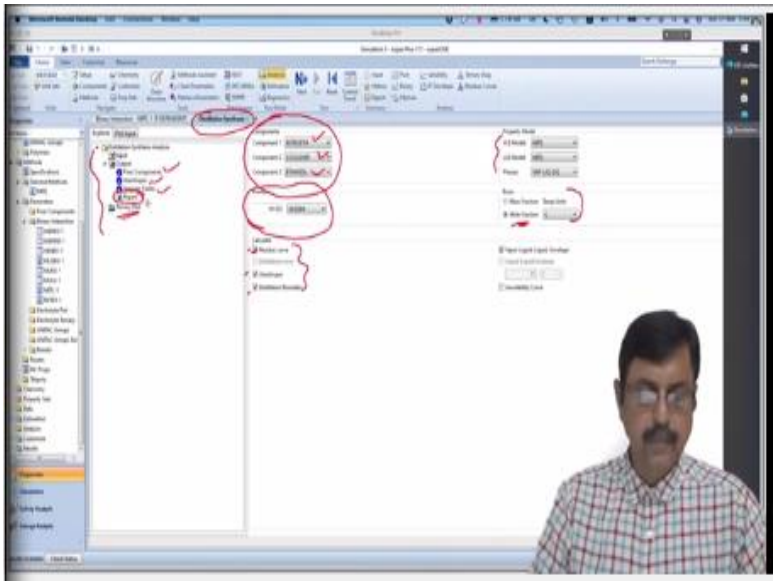

So, we press it and then we get this particular distillation synthesis and here we have several information. So, the component list has been given, so component 1 is nitroethane, cycloheptane is component 2 and ethanol is ahh component 3. And the analysis is done at pressure which is 1 atmosphere the VLE, LLE the model is NRTL. And basis is mole fraction not mass fraction and temperature is calculated in centigrade unit.

So, they will calculate residue curve, azeotrope and distillation boundary. Now we have ticked all of them because we want them to calculate all of them. In case you do not want to see the residue curve you can untick this or if you do not want either of them you can untick this, so that is up to your convenience. And the left-hand side, you will find this explorer where you can get the output in pure component form or azeotropes, singular points, generate a report, and see the ternary plot.

Now let us go to the pure component first, let us see what they are? So, it says stable node, so pure component stable node is the boiling points of nitroethane, cycloheptane and ethanol, respectively. If you want to check, you can check here just go to internet and write nitroethane and you can see the boiling point is 114 °C.

Similarly cycloheptane you will find 118.8, it is 118 point well it has calculated as 1 probably this is the experimentally found one. And it has been calculated through NRTL method, so that kind of difference may be observed. And ethanol it is 78.31, let us see what internet says, ethanol, it is 78.37, 78.31. So, stable node is the boiling point of these liquids at 1 atmosphere,

mind that we have calculated it as 1 atmosphere, if you change this value, then the output will also change.

If you change it to 2 atmosphere or 3 atmosphere or some other pressure then the stable node the values will change, the boiling point will change, that information will change. There are four azeotropes you get, three are binary azeotropes, you will find the binary azeotrope over here.

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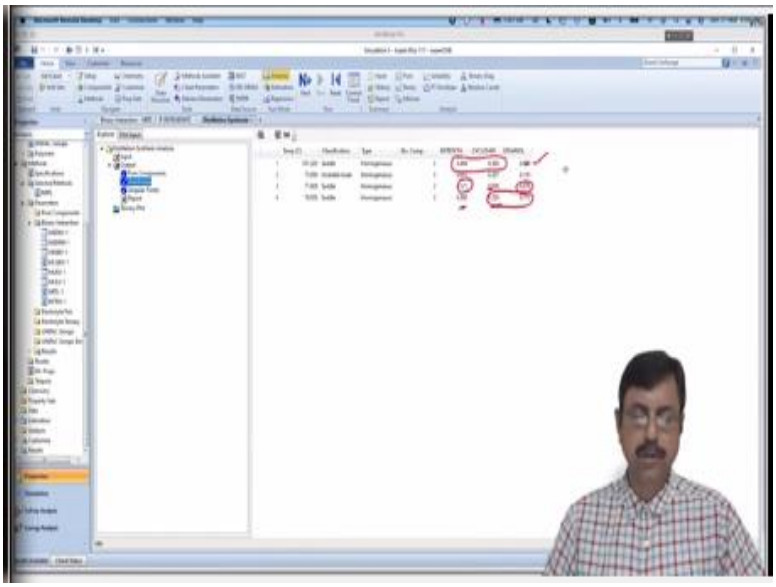

So, this is the first one is the binary azeotrope, it is an azeotrope between nitroethane and cycloheptane, the third one is a binary azeotrope between nitroethane and ethanol and the last one is a binary azeotrope between cycloheptane and ethanol. All these three we have one of the components missing, so they are binary azeotropes.

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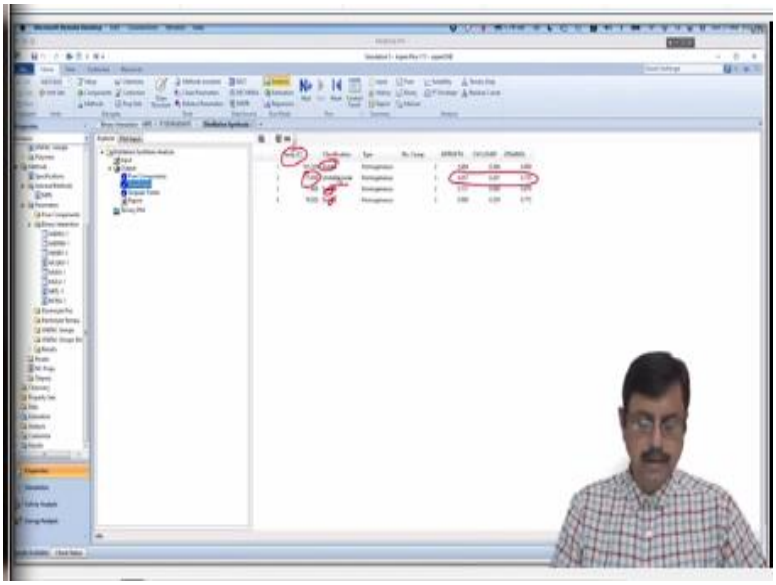

We have only one azeotrope over here, that is ternary azeotrope, which is at 75.7589 °C, and obviously, this is unstable node. And, these are saddle node because if you see the ternary plot and residue diagram you will see why it is called saddle point or saddle node. Similarly, you can see the singular point; singular point is nothing but the collection of all stable, saddle, and unstable nodes.

Therefore, it is collection of all the boiling points and the azeotropes. Finally, the report if you press report then nicely generated azeotropes search report will be given, you will find here the mixture investigated for azeotropes at pressure 1 atmosphere, the component id, component name, classification, the temperature everything will be given. There were there were 4 azeotropes, you will find all those 4 azeotropes over here, their temperature.

Finally, this is the ternary plot, so in ternary plot this one is the ternary azeotrope; this is a mixture of 3 points. In addition, these are the 3 binary azeotropes and these are the stable nodes along with the boiling point. So, this information is given, cycloheptane 100% with boiling point, this node is 100% nitroethane with this boiling point and this node is 100% ethanol with this boiling point.

In addition, the mole basis information will be available when you have this mouse on the graph, it will tell about corresponding mole fractions, compositions of the ternary mixture.

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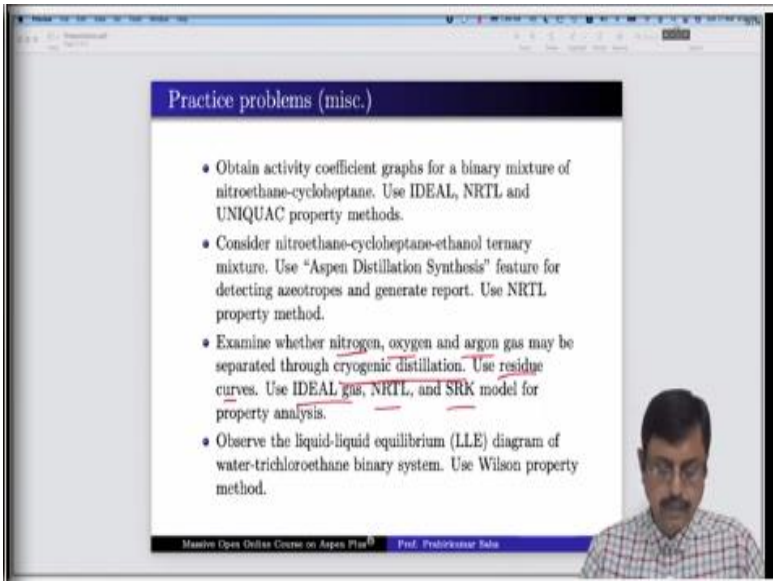

So, that is how we use the "Aspen Distillation Synthesis" feature for detecting azeotropes and to generate report. Now our next problem is examining whether nitrogen, oxygen and argon gas may be separated through cryogenic distillation. Cryogenic distillation means the distillation that is done below 0 ℃. Now at normal temperature all these components like nitrogen, oxygen or argon all of them are gas, so their boiling points are much below 0 ℃.

So, we have to see whether they can be separated through cryogenic distillation and we will examine it using the residue curve. And for that we shall use IDEAL gas method, NRTL method and SRK model for property analysis. So, for that let us open the Aspen simulation window. **(Video Starts: 22:33)** So, write the components nitrogen, oxygen and argon, press Next. And we have 3 methods IDEAL, NRTL and SRK IDEAL, NRTL and SRK, run the property methods, run them twice or thrice as many as times it wants. Ok

Now they are done, there is an error; I know what the error is. Actually when you are using SRK, method then you have to use free water method as steam NBS and that is exactly what the run status should say. Let us check, yes, free water method should be steam NBS when main property method is SRK, so that is the common mistake people do. So, we have to check it with steam NBS and run, yeah now the run status is ok. Now we have to bring the residue curve, nitrogen, oxygen, argon, first the property method IDEAL, ok so this is with IDEAL curve let us bring another residue curve. Let us use NRTL ok and let us bring the third residue curve and that is using SRK. Ok

So, now basically we have 3 residue curves, the first one it has been generated using IDEAL property method. The second one has been generated through NRTL method and third one has been generated through Readily Quanks Wave method. And we find none of them are showing any kind of azeotropes, ok so only the experimental investigation will tell you which method will be most ideal for this kind of situation.

But why we have tried 3 methods because the first one is IDEAL method, the second one is NRTL, so it is activity coefficient based model and the third one is Readily Quanks Wave method (26:33) model, this is equation of state based model. So, all 3 types of modelling technique we have tried and none of them are showing any sign of any kind of azeotropes. **(Video Ends: 26:50)**

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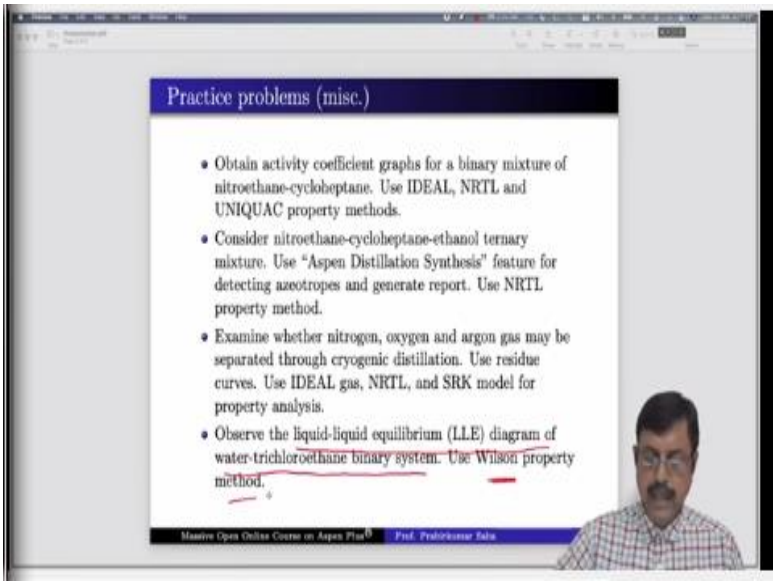

So, the answer to the question, which has been asked, examine whether this gas may be separated through cryogenic distillation? The answer is yes, it is possible to separate them through cryogenic distillation. Then the final practice problem that we have it is about observing the liquid-liquid equilibrium diagram of water trichloroethane binary system using Wilson property method. So, for that let us again go to the Aspen simulation window and open a new simulation. Ok **(Video Starts: 27:31)**

So, we enter water then trichloroethane, ok we choose the first one, so we have to rename it as TRC, press next we will use Wilson method. And we shall estimate using UNIFAC otherwise this particular parameters are not being calculated, so run them. Now we have to see the liquid-

liquid equilibrium diagram and let us say binary water TRC at 1 atmosphere pressure, Wilson method, run analysis.

So, this is the diagram that we have and if you check the VLE y versus x and you will find like this. So, basically this is a liquid-liquid diagram basically water and trichloroethane they do not mix with each other, they have poor solubility. **(Video Ends: 29:35)**

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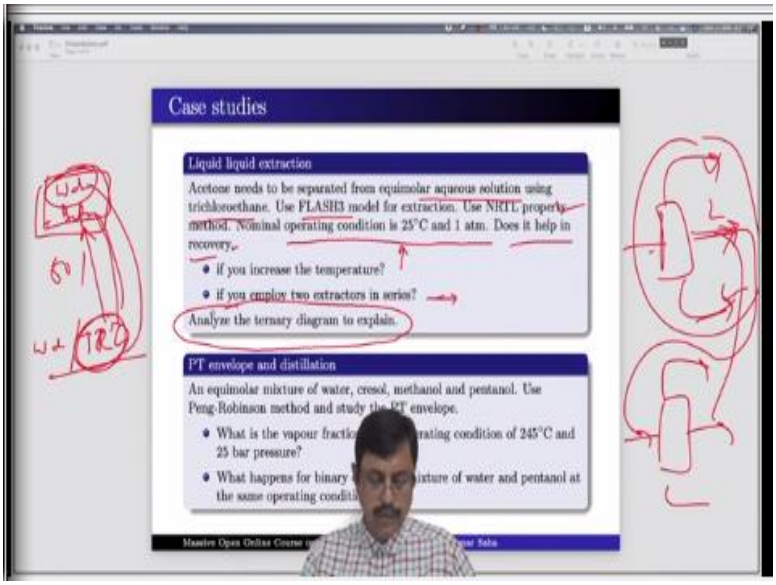

Now we will perform 2 case studies, there will be a bit detail and we will see more information in this. The liquid-liquid equilibrium that we have just seen the same problem will be extended in that the first case study.

Here acetone needs to be separated from equimolar aqueous solution, that means we have a solution where we have water and acetone and they are equimolar 50-50 and we have to use trichloroethane to extract. Therefore, as we know water and trichloroethane they are not miscible at all that we have seen in the previous practice problem. So, we expect that TRC when we mix with this water, acetone mixture then TRC will take out the acetone from here. So, it will extract the acetone from that mixture.

Because acetone mixes with water, acetone mixes with TRC but water and TRC they do not mix with each other, so this can be used for extraction. We will use the FLASH3 model for extraction because we know FLASH component it has vapour and liquid but FLASH3 it is vapour-liquid-liquid. So, there are 2 liquid outputs we have in FLASH3 model, so we can use it for extraction.

We will use NRTL property method and the nominal operating condition is 25 ℃ at 1 atmosphere pressure? So, it is normal operating condition. Now 2 questions have been asked, does it help in recovery if you increase the temperature or if you employ 2 extractors in series? That means one FLASH3 which is in series with another FLASH3 that means the output of this will be added into this.

So, whether this kind of system will help to get more recovery of acetone? Now we have to analyze this using the ternary diagram and we have to explain. So, for that let us go to our Aspen simulation window. **(Video Starts: 32:18)** We will not open the new simulation window, we will use this one only because we have to just add one component that is acetone.

So, we already have water and TRC, so we we add acetone and we shall use NRTL method. Now we have to analyze with ternary diagram to explain, we will do it later. First let us see what happens for this kind of system, ahh let us simulate the system first. So, let us go to the simulation window, bring the FLASH3. So, add the material first, so this is the feed, this is vapour, this is liquid 1, this is liquid 2.

So, this one we have to reconnect source this one. So, this is feed, this one is vapour, well ahh actually we will not get any vapour in this because at normal temperature and pressure condition none of this water, TRC and acetone none of them have any vapour phase. But Aspen has to have some line with it obviously it will go dry after the simulation, does not matter but we have to set this line vapour line.

And here we have to press liquid 1 and this is liquid 2, ahh we will use V instead of vapour. ok So, press next, it is 25 ℃ and 1 atmosphere pressure and it is an equimolar mixture of water and acetone, so it is water and acetone equimolar. And in the flow sheet we have to have a second stream, that is TRC stream. So, we add in the second stream over here and that we call TRC stream where you have only TRC of 1, 1 atmosphere that's it.

So, press next, ok so the flash tank let us run it at 25 ℃ and the same pressure 1 bar. So, now it is ready to run, let us revisit the main flow sheet we have a feed which is equimolar 1 kmol/hr of water and 1 kmol/hr of acetone, so it is an equimolar mixture. And we are sending 1 kmol/hr

TRC into it, it is flashed, vapour will go dry because it is at normal temperature and pressure, we will get 2 lines of liquid, liquid 1 and liquid 2.

Because one will get the extract, the another will get the raffinate. So, now let us run, ok so we have run the simulation, go to the stream result and this is the stream result that we have. See the molar flow rate, we have out of 1 kmol/hr, we have got 0.87652 kmol/hr in the L1 TRC is very small and we have got 11% or 0.1122 kmol/hr acetone over here in the raffinate phase.

In the extract we will have almost entire TRC and we will have 88% of acetone going to the extract phase. ok So, let us write this information

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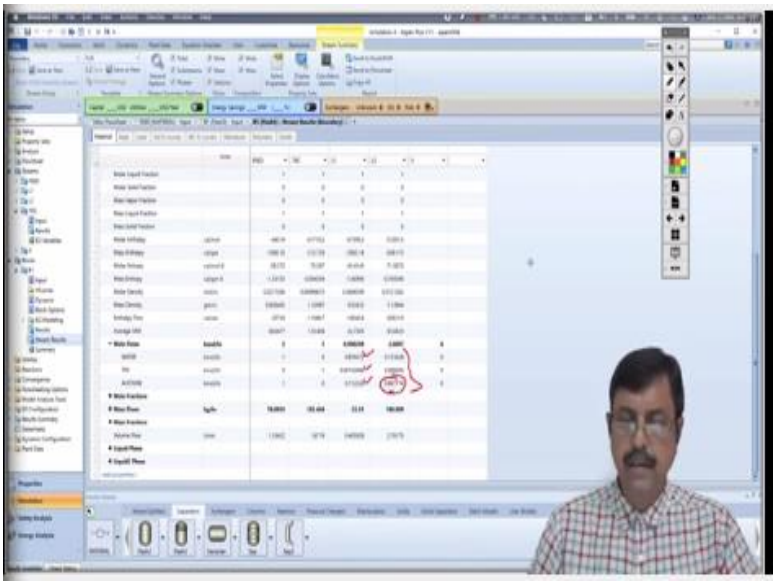
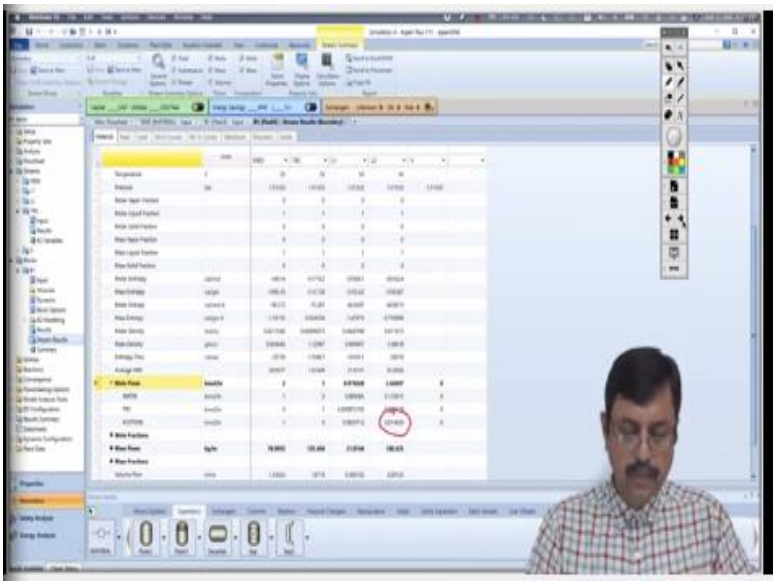


So, we have we have to remember this information L1 (Water- 0.876572 kmol/hr; TRC- 0.0015 kmol/hr; Acetone- 0.1122 kmol/hr). And we also have to remember the amount of heat duty, let us use it in SI unit. So, it is nearly 1 kilowatt, 1.073 kilowatt, this is the amount of heat duty that is required for running the system. Now we keep this information with us, let us increase the temperature.

So, the first problem if you increase the temperature can you get a better result? For that let us increase the temperature to 50 ℃. Suppose we increase the temperature from 25 ℃ to 50 ℃, what happens? Let us run it once again, we see the heat duty in this case is 3.9257, so from 1 kilowatt, it is going to 3.9257 kilowatt almost 4 times the energy requirement is there for an increase of temperature from 25 ℃ to 50 ℃. Ok

But are we getting a better result? See the stream results, so these are the stream result we have in the mole flow rate, check the mole flow rate, here we are getting acetone 91%, so let us check. So, here it is here it is 91.49% recovery of acetone by using 50 ℃. But what happened for the previous 2 cases? It was 88.7744% of acetone, so you are spending 4 times of energy just to increase it from 88.77 to 91.49. **(Refer Slide Time: 41:55)**



So, only 3 or 4% increase your energy requirement will be 4 times higher which may not be advisable. Now the second option is saying if you employ 2 extractor in series, let us change our flow sheet a bit. So, here we bring in another FLASH, so this is our second V, this is our L1, L2 and then this needs to be connected to this one and we need another TRC over here. So, this one we name it TRC2, this is V2 which again will go dry, let us say this is L1 dash and this is our L2 dash. Ok

And we will mix up 2 extracts together, so that our calculation we do not have to do separately. So, for that we connect this thing over here and this one we reconnect destination to this. ok So, we have 2 connections, 2 inputs and 2 outputs ok ok and the total of extraction it is this one, we write total. So, we will check what the composition of the total stream is? And we will not send the entire 1 kmol/hr over here, we will distribute it 0.5, 0.5, so we will distribute it.

So, let us say TRC is 0.5 and TRC2 it is again 25 ℃, 1 atmosphere pressure and this is 0.5. And the blocks B1 we reduce to 25 ℃, we do not want any major change in pressure, ok temperature 25 and pressure 1 atmosphere. Now let us run, ok now we have to check the stream

result of B3 because it will give us the output total. Now you check what is the output in B3? Here we see the amount of acetone is 0.96, so 96%.

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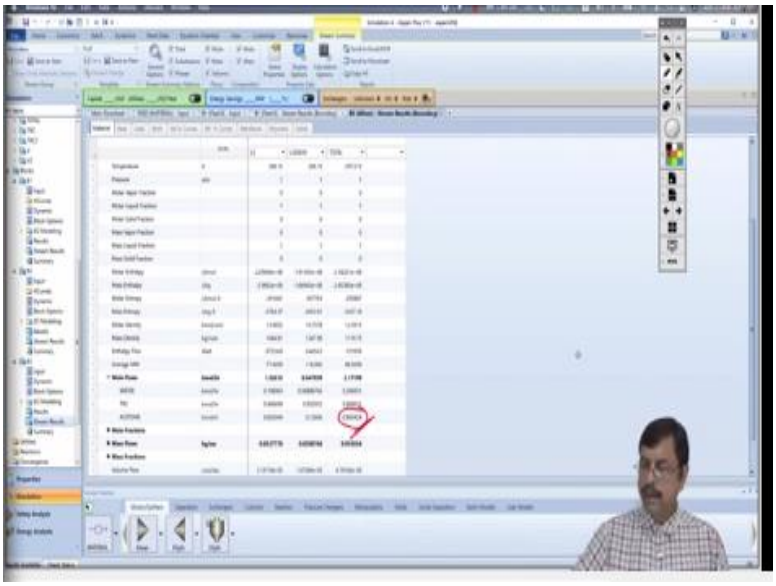

So, from 88.77 to 96.54, so we have increased the extraction capability of the unit by adding another extractor in series. And what is the heated duty? So, heat duty will be 308 watt and B1 712 watt. So, 700 and 800 nearly 1.5 kilowatt, so earlier it was 1 kilowatt now it is 1.5 kilowatt by keeping 2 extractors in series we are increasing the heat duty by 50%. But we are extending the purity of acetone from or extraction of acetone from 88% to 96%. To add an extra unit, you obviously need a capital cost, but your recurring cost that is hit heat duty will be lower.

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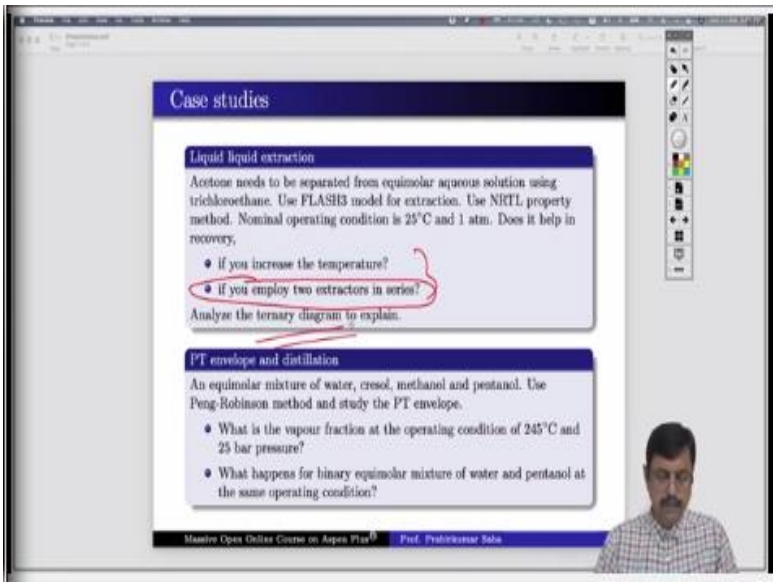

So, if you are given 2 options like this, then obviously this option is better. Now we have to analyze the situation using ternary diagram. **(Video Starts: 48:53)** We have to go back to the property method and check the ternary diagram, run analysis, it is something like this. Let us increase the number of tie lines, so make it 15 tie lines, yes. Initially, it was equimolar right, because in the B1 mixture, it was 1 kmol/hr of water, 1 kmol/hr acetone, and 1 kmol/hr TRC. we I am not talking about 2 extractors in series, I am talking about the case where we were using single extractor.

In that case inside the extractor it was truly an equimolar composition. Equimolar composition means the location of composition will be somewhere here because here it is equimolar point.
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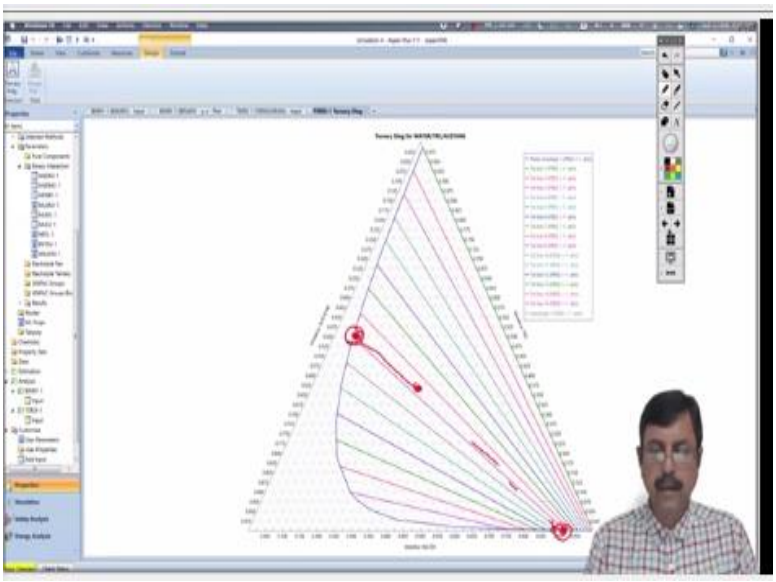

Now if this is the equimolar point then any kind of extraction will go one phase at this point and one phase at this point, ok so that is how the extraction works.

Now you can check the composition of extract and raffinate phases you will see them this point and this point. For instance, this is the point where water is released so it is the composition of L2. On the other hand this is the composition of L1 where we will have almost no TRC, TRC is almost 0, ahh it will be ahh nearly 91 or 92% of water and very small amount of acetone, so let us see. So, here almost no TRC water is nearly 90% and acetone is very, very small.

So, that is how you can analyse the ternary diagram and check whether your simulation results match with whatever you examine through the ternary diagram.
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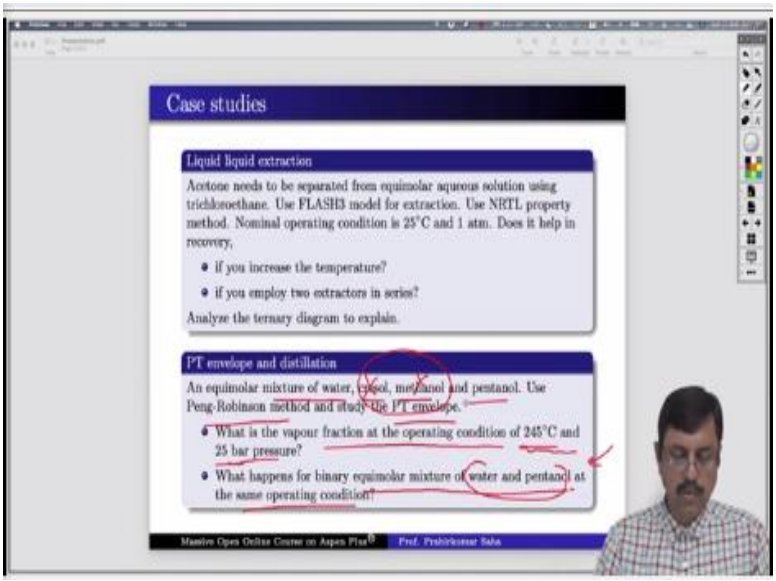

So, our second case study is about PT envelope and distillation. So, it is about an equimolar mixture of water, cresol, methanol and pentanol, we have to use Peng-Robinson method and study the PT envelope.

Now 2 questions are asked, first question is what is the vapour fraction at operating condition which is 245 ℃ and 25 bar pressure? And what happens for a binary equimolar mixture of water and pentanol? That means that we will have only water and pentanol in the second condition, there will be no cresol, and there will be no methanol. At the same operating condition, the operating condition will still be 245 ℃ and 25 bar pressure but in the absence of cresol and methanol.

So, this is the case study that we have to perform. For that let us go back to our Aspen simulation window. **(Video Starts: 53:41)** So, add water, cresol, methanol and pentanol, ok press next, use Peng-Robinson, press next, ok run. Ok Now the first task is study the PT envelope, so let us bring in PT envelope, now let us take equimolar flow rate that has been asked.

Equimolar mixture of water, cresol, methanol, and pentanol is 1, 1, 1 and 1 and run analysis. So, this is the PT envelope we have got, but we have only 2 lines one is vapour fraction1, the blue line, this is the dew point line and vapour fraction 0, this is the bubble point line. But we may not be happy with only 2 lines we need some more lines for analysis.

For that, let us add additional vapour fraction line at say 0.2, 0.4, 0.6 and 0.8. So, run the analysis once again, yeah so we have few more lines like this. So, we just shift it over here, so each line the legend is also given, so you can check the legend and find out which line corresponds to what? Now question is what is the vapour fraction at operating condition 245 ℃ and 25 bar pressure?

So, it is 25 bar pressure, so 25 bar pressure means 25 bar pressure means this line and 245 ℃ means this line. So, this is the point we are looking for, ok, so what vapour fraction it is? This is a gray line, so I think it is 0.4, yeah, so this is 0.4 line. ok So, our condition is over here this is the point. That means if we run the distillation at 25 bar pressure and 245 ℃ then the 40% of the feed will go into the vapour phase that is what it means.

So, let us cross check, go to simulation and bring in the separator, FLASH, material in, this is vapour out, this is liquid out, this one we reconnect to destination. Rename, this is my feed, this is my vapour and this is liquid. Next, it will ask for input streams, so 245 ℃ and 25 bar pressure and all of them are 1 equimolar mixture of all of them, press next, ok block again 245 ℃ and 25 bar pressure, run the simulation, yes. So, see the stream results, so molar flow it is 4 kmol/hr. But what is the vapour fraction? It is 1.5734.

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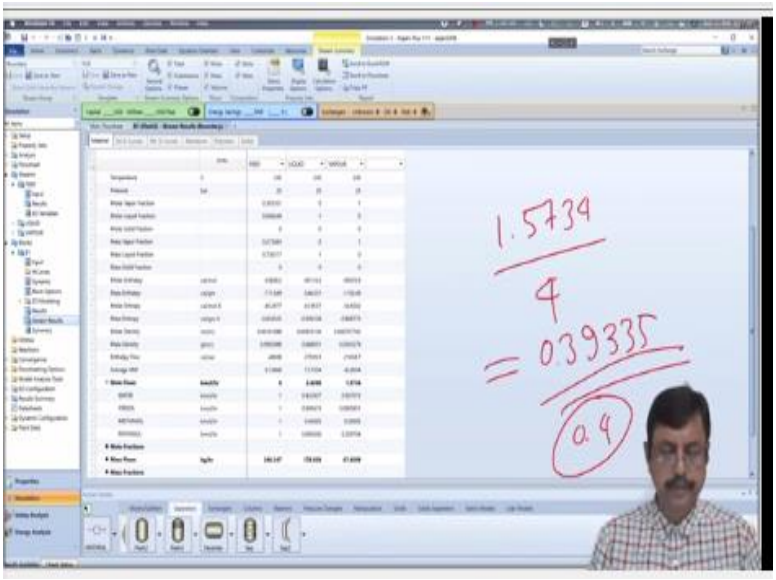

So, 1.5734 by 4 So, 1.5734 by 4 that is equal to 0.39335 which is near nearly 0.4 and this information we have obtained from PT envelope. Ok Now thus next question is what happens for binary equimolar mixture of water and pentanol at the same operating condition? That

means we shall check out this cresol and methanol only water and pentanol will remain, it will be equimolar mixture.

So, for that let us go to the feed input and we check out this cresol and methanol Ok and we run the process. See the results and we find in the molar flow, we do not find anything in the liquid.

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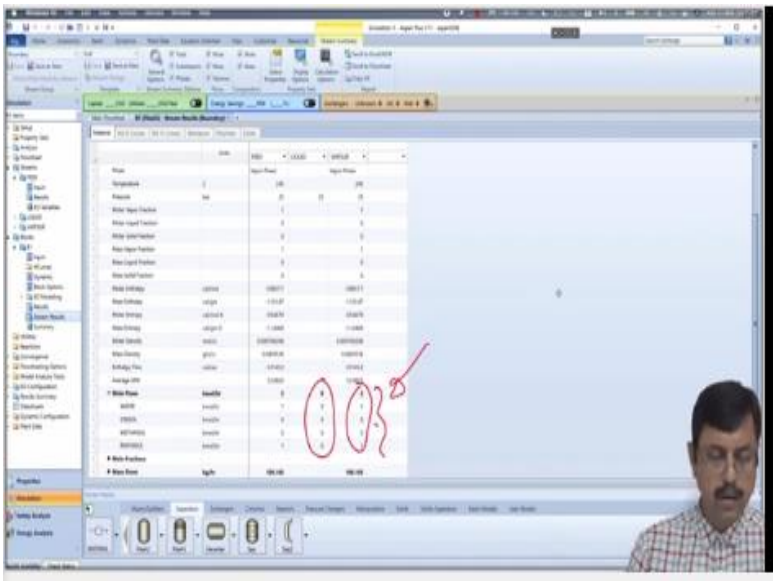

Here we do not find anything in the liquid phase everything has gone to the vapour phase. ok So, this is an interesting result that if we check out cresol and methanol then at the same operating condition everything will go into the vapour phase, nothing will remain in the liquid phase.

Now let us crosscheck this with the PT envelope. For that let us go to the property analysis, the PT envelope, here you delete this one, delete this one and run the analysis once again. Now the curves are a bit different, ok so let us analyse this curve. Now what is the condition? It is 245.

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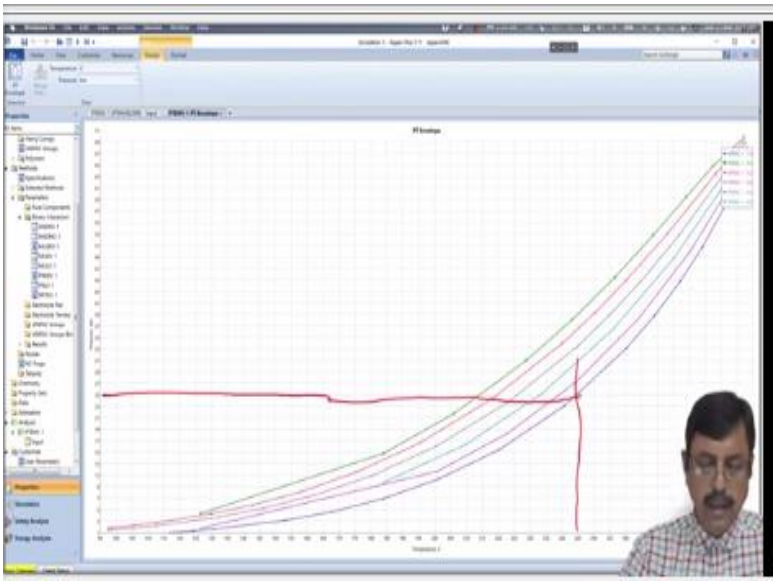

So, 245 is here this line and what is 25? 25 bar pressure it is this line, so this is the point. Now check it very closely this point where my mouse is hovering around, this is just outside the vapour fraction 1 curve, it is not within this.

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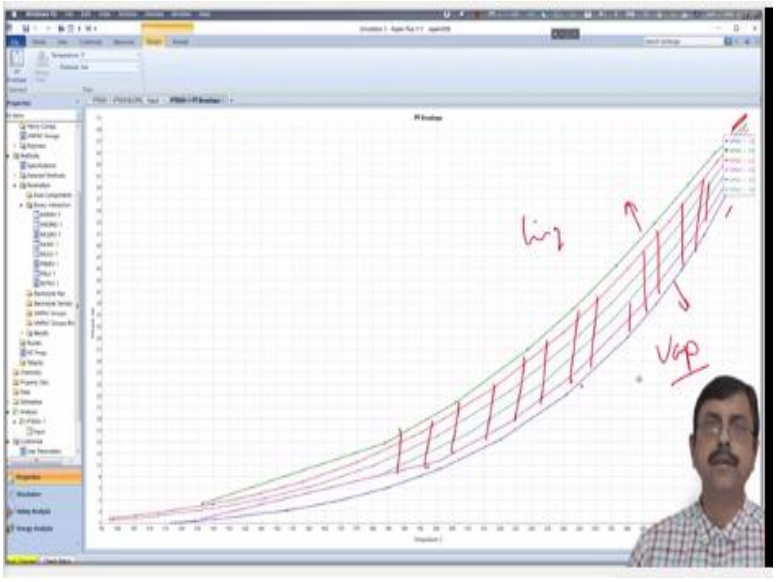

So, anything that is of this side will be completely vapour, anything this side will be completely liquid. Only between these 2 vapour lines, vapour line 0 and vapour line 1 within this there will be a liquid and vapour mixture. ok So, in this particular case when we are driving cresol and methanol out of our system then for the same operating condition it is bringing the system into the completely vapour region. Ok

And as it is coming at the completely vapour region we are not getting anything in the liquid. Now let us change the temperature from 245 ℃ to 240 ℃ and let us check what happens.

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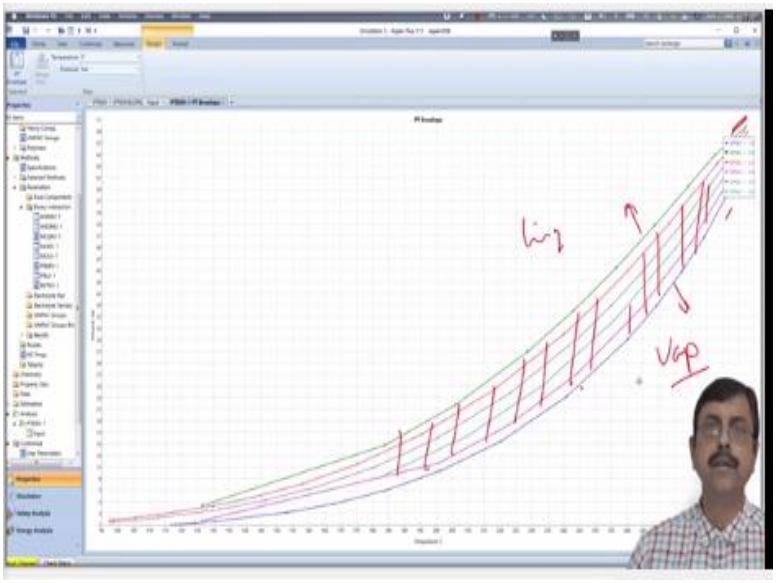

Mind that this is near the curve 0.8, 0.8 vapour fraction. So, if we change our temperature from 245 ℃ to 240 ℃, keeping our pressure constant at 25 bar.

Then we were expected to have a vapour fraction of 80% nearly, let us check that. So, go to our simulation once again, here in the feed we make it 240 ℃ and the B1 also keep it 240 ℃ and run the simulation once again. Now see the stream results, here you will find what the vapour fraction is?

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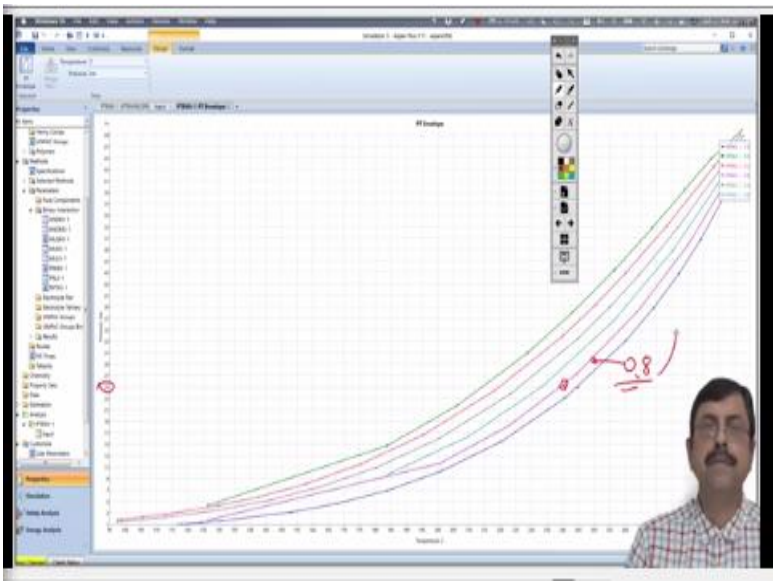

Vapour fraction is 1.62763, so the liquid is not going completely dry this time. And what is the amount? It is 1.62763 by 2, which is around 0.8138 ok nearly, point nearly 81.38% and that information matches with our observation in the PT envelope curve. **(Video Ends: 1:08:56)**

So, in today's lecture we have performed 4 practice problems of miscellaneous in nature and we also have done a couple of case studies. So, with this we end our lecture today, we will continue in the next lecture. Thank you.