Aspen Plus Simulation Software – A Basic Course for Beginners

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Lecture-18
Practice Problems on Binary Mixtures

Welcome to the massive open online course on Aspen plus.

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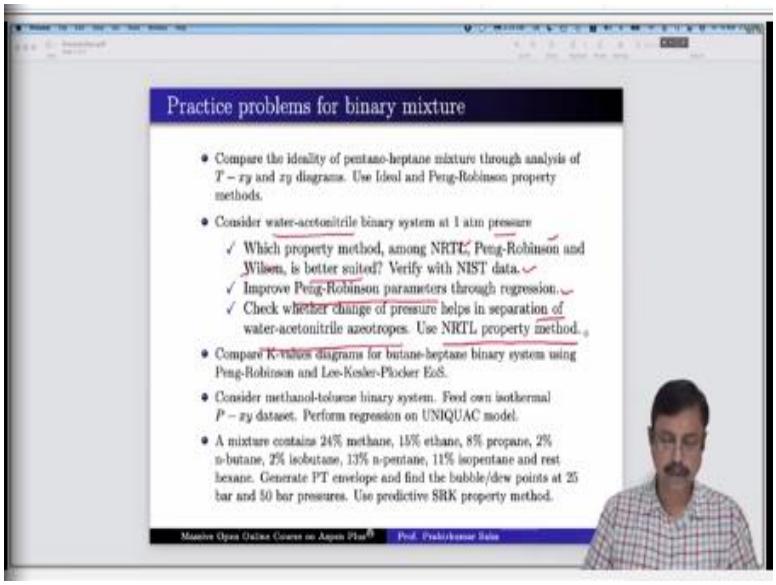

In today's lecture we will perform some practice problems on binary mixture. In that last lecture we have done the practice problems on pure components, today we will do on binary mixtures. All together we have 5 problems to solve; the first problem is about comparing the ideality of pentane heptane mixture through analysis of T xy and xy diagrams. And we will use ideal and Peng-Robinson property methods. For that let us go to the Aspen plus simulation window.

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So, here we have to first enter the components which are pentane and heptanes. And we shall use the ideal method as well as Peng-Robinson method. So, let us run the property method, yeah, the property methods are run. Now we have to bring in the binary mixture, so we brought the binary analysis tool. Here we have pentane and heptane for pressure 1 atmosphere, the calculation option is Peng–Robinson.

First let us do with ideal method; we will do Peng-Robinson later. So, for ideal method if we run the analysis we obtain this particular curve. Now let us change it to lines only, do not use marker and we write ideal because later we have to distinguish it from Peng-Robinson method, so binary plot is done. So, now we will bring in another binary analysis and in second binary analysis everything will remain same only the calculation option will change.

In the previous case we did it with ideal property method and this time we will do it with Peng-Robinson method. So, let us run the analysis once again, so this is the T xy diagram for pentane and heptanes when Peng-Robinson method is used. So, here again we use only lines not markers and we change it to Peng-Robinson and Peng-Robinson over here. So, this is the diagram for Peng-Robinson method and this is the diagram for ideal method and this is the diagram for Peng-Robinson method.

And let us merge the plot and check, yeah, we have merged the plot and we can take everything in the single axis. We find that the results obtained by using ideal method and results obtained using Peng-Robinson method they almost match with each other. The curves they superimpose on each other, the bubble point curve almost exactly match with each other and there is slight difference in the dew point curve but that is acceptable. So, now let us check the x y diagram, so this is the x y diagram for Peng-Robinson method. And for binary one let us bring the y versus x curve; this is for ideal case.

So, we use only lines and here also we use only lines. Now we merge the plot, so here again we merge the axis, so we observe that for y x diagram, that is y x, vapour liquid equilibrium diagram. The result obtained through ideal property method and the result obtained through the Peng-Robinson method both of them they almost superimpose on each other. The error is or the difference is very, very minimum. So, from this analysis we can conclude that pentane, heptane binary system is nearly an ideal system, the non-ideality is very, very minimum.

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Now we go to the next problem, here we have a water acetonitrile binary system at 1 atmosphere pressure. Now we have to do 3 tasks over here, there are 3 property methods suggested NRTL, Peng-Robinson and Wilson. We have to check which is better suited and this information we have to verify with the NIST data set. And we will expect that Peng-Robinson parameters will not be very good because water acetonitrile binary system at 1 atmosphere pressure will be mostly liquid.

So, activity coefficient model will be better suited. So, for that matter NRTL and Wilson method they are expected to perform better and Peng-Robinson method perhaps will not perform better. So, we have to improve the Peng-Robinson parameters through regression, so that its performance comes to an acceptable range. And then the 3rd task is we have to check whether the change of pressure helps in separation of water acetonitrile azeotropes.

Now here we will expect that the system will have an azeotrope and if we need to perform distillation in order to separate water and acetonitrile, then changing pressure whether it will help. So, that we have to check and for that task we have to use NRTL property method.

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So, for that we have to go to aspen simulation window and we will open a new simulation. So, we enter the components, first is water and then we will have acetonitrile.

So, this is the one which we are looking for, add selected components, we rename it to acetonide. Next, so we have 3 property methods NRTL, Wilson and Peng-Robinson, so these 3 methods we will operate. Now let us bring in some NIST data. So, we have binary mixture for water and acetonitrile, let us retrieve the data first, this may take a few minutes depending upon the speed of internet**.**

So, we have got some binary VLE suppose we choose the first one, so it is VLE 001, the liquid mole fraction, water and this is the temperature in Kelvin and this is the vapour mole fraction of water and this is the pressure. So, pressure is 101325 N/m^2 that means it is 1 atmosphere pressure. So, let us save this data, so we will go to the data set**.** Now this data type as we have the

pressure data, so aspen is assuming that pressure is changing so it is showing it as a T P xy data table.

But we understand that pressure is constant at 1 atmosphere, so what we will do? We will change it to T x y in place of T P xy, in that case we have to add some constant temperature of pressure data over here. So, we will change it to T xy and we will write over here 101325. Now in the data set the pressure column disappears. Now let us check that T xy diagram, so this is the T xy diagram we have, so this is the experimental value of T xy data for water acetonitrile system.

The blue dots are the vapour mole fractions and green data, green squares there of x that is the mole fraction of water in the liquid. So, both of them are mole fraction of water not acetonitrile. Now what is the temperature range? The temperature range is 348 to 374. Now let us go to the binary analysis. For that let us bring in binary analysis tool this is the T xy diagram and we keep it at 1.01325 bar because this is the pressure at which the experimental data has been changed. So, first we will do with NRTL, so run analysis.

Here we change it to lines only and change it to Kelvin because the experimental data are there in Kelvin. So, if we have to compare it with experimental data we have to change it with Kelvin. And here we write NRTL because later we have to distinguish it from others. So, now we bring the second binary analysis tool and here everything will remain same only the calculation option will be different, it will be with Wilson rather than NRTL.

So, we will run the analysis once again, so we get another result, we just keep the lines not the marker, we change it to Kelvin and then we write Wilson over here, Wilson, done. So, we have got the T xy plot using NRTL method and then we were using with Wilson method. And the third one again we will bring another binary analysis tool and this time we shall use Peng-Robinson method.

Run analysis, so visibly this curve is not acceptable, anyway just change it to lines and then bring over here Peng-Robinson, Peng-Robinson again, done. So, binary 2 plots it is Wilson and binary 1 it is NRTL. Now we have to combine all these curves and check. So, this curve we merge the

plot with binary, binary 3 also we merge with binary 1 and the experimental data that also we merge with binary 1.

So, actually the binary 1 curve now it has 4 curves, so all of them we have only the lines not the markers and we shall change the axis to single axis. Now you can see the experimental curve this one, we keep line and marker or we can keep marker only because this is the experimental curve and then the other one that is blue line this one, we keep marker. So, now we can see the experimental data and the T xy diagram obtained by using 3 property methods NRTL, Wilson and Peng-Robinson.

So, visibly we can see the 2 methods like NRTL and Wilson they are able to come near the experimental data. They somehow are trying to match the experimental data but the Peng-Robinson method it fails miserably. Now it is expected because Peng-Robinson method is equation of state method not activity coefficient.

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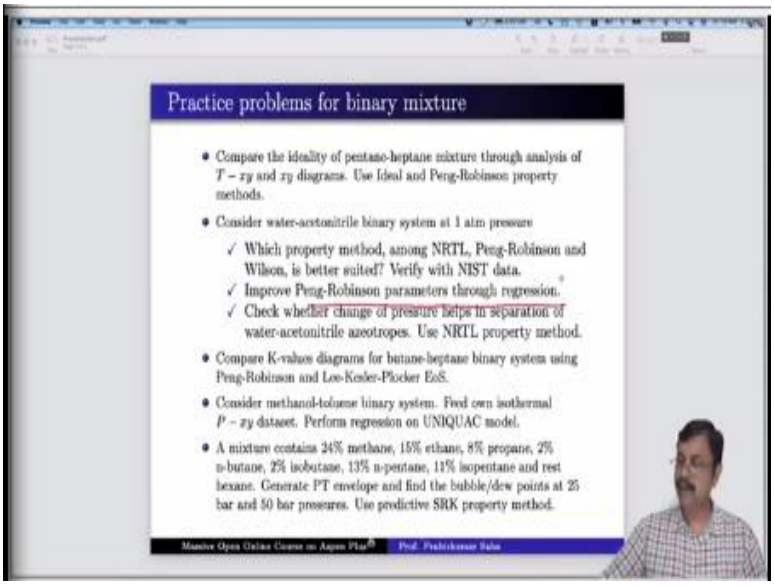

But here we have the next task; we have to improve the Peng-Robinson parameters through recreation. Now we have deleted all other things like NRTL and Wilson method we have deleted, we have just retained the T xy diagram obtained through Peng-Robinson method and

that we are comparing with the actual experimental data obtained from NIST. And this is the result that we have getting.

The solid lines they represent the simulation result obtained through Peng-Robinson method and the red dots are y experimental mole fraction. And the magenta squares they are experimental data for mole fraction of water in the mixture of water and acetonitrile. So, this one we keep now for the time being and we want to improve the Peng-Robinson method. So, next task is, improve the Peng-Robinson parameters through regression.

So, that the; improved Peng-Robinson method can match with the experimental data, that we have got. For that we have to do the regression, so let us bring in the regression over here. So, press new, the new id and the data set we have only one data set over here and the parameters. So, first let us check the binary parameters and we will choose PRKBV that is the binary parameter vector for Peng-Robinson equation of state the KIJ.

So, let us use it is first element component water and acetonitrile and let us run the regression. So, it has run, now let us run the binary analysis once again with the improved Peng-Robinson method. So, this is the binary curve and this is the result that we have got, earlier at least this portion was here. So, actually the model got worse after regression, so we have only regressed one parameter, so that might be the reason.

So, the next time what we will do? We will increase the number of parameters, say we shall regress, this one and then we will regress, this one and regress, another one which is mu. Let us see whether we get a better result with them? So, run the regression once again, so yes to all, so all of them have been changed now and this is the updated curve. Now it is much better, the green and blue lines they are model output simulation result through improved Peng-Robinson.

And the dots and squares they are experimental data this result is much improved once. So, we can conclude that by changing 4 parameters the Peng-Robinson method becomes better. So, I believe that if you increase one more parameter or 2 parameters then the result will be much better.

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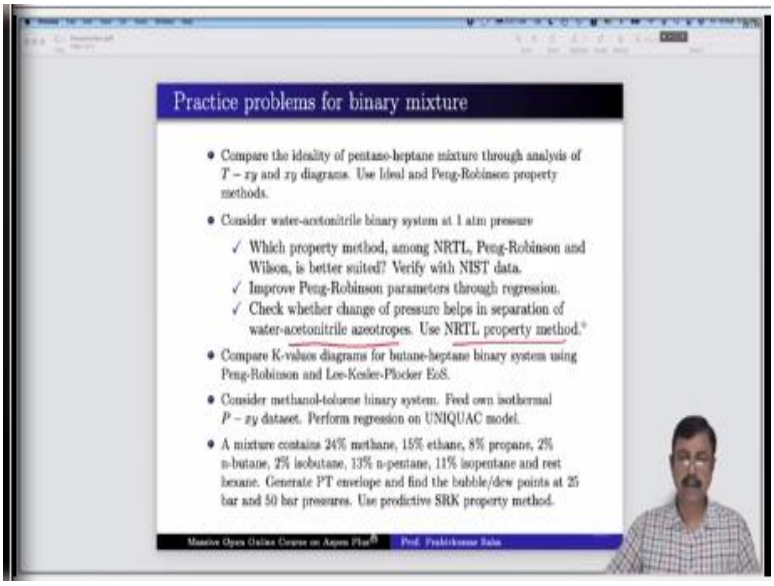

Our next task is to check whether change of pressure helps in separation of acetonitrile azeotropes, we have to use NRTL property method.

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Now if we check the curves we will find at this point we have some azeotrope. So, if my system has 27.5% of water and rest is acetonitrile then we will not be able to separate them through distillation because that combination forms an azeotrope.

Now we have to check by changing the pressure of the system whether it helps? So, for that we have to use NRTL method that we have done, so we will use NRTL method over here. Now whether or not change of pressure helps we shall not analyze it in with one pressure rather we will analyze it with multiple pressures. So, let us analyze it at 1 atmosphere pressure, 5 atmosphere pressure, 10 atmosphere pressure and 25 atmosphere pressure.

Let us check 4 pressures and see how the T xy diagram looks like. So, run analysis, so this is the diagram that we have got, this one is 25 atmosphere pressure, this one is 10 atmospheres, this one is 5 atmosphere and the last one is 1 atmosphere. So, as you can see that as the pressure

increases the temperature also increases, so that is expected. Here one thing you can notice that at 1 atmosphere pressure the azeotrope lies somewhere here.

If we increase the pressure up to 5 atmospheres then the azeotrope shifts, with 10 atmosphere it further shifts and with 25 atmosphere it shifts again. So, if your; binary mixture contains say 30% water and 70% acetonitrile then obviously with this composition at 1 atmosphere it is not possible for you to separate through distillation. But same thing is possible at 25 atmosphere pressure, because at 25 atmosphere pressure this mixture condition is no longer an azeotrope. So, it has separate bubble point and dew point, so it is possible for you to separate through distillation.

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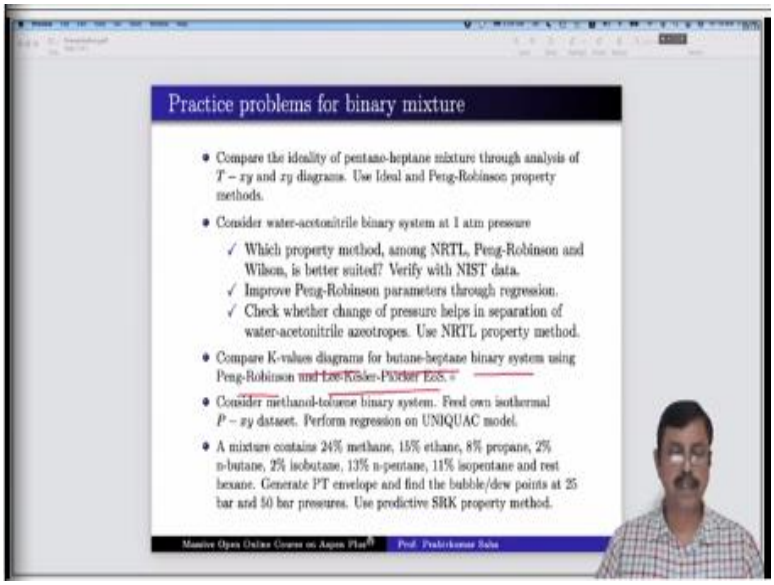

So, the answer to the query that has been asked in the question whether, change of pressure helps a separation of water acetonitrile azeotrope? The answer is yes, it helps. So, our next problem is comparing K values diagram for butane heptane binary system using Peng-Robinson and Lee-Kesler Plücker equation of state. So, for that again we have to go to the aspen simulation window.

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Let us open a new one, so the components are butane and heptanes, so we have Peng-Robinson method and Lee-Kesler Plocker method, run those property methods, we are done. Now we have to bring K value diagram and for that we have to do the binary analysis. So, first we are doing with Lee-Kesler Plocker, so we cannot directly bring the K value diagram, first we have to do it with T xy that is what aspen does.

So, we run the analysis first with T xy and when it is over the K value diagram will be available. So, here we are not interested to know about T xy diagram, we can bring the K value diagram from there. So, this is the K value diagram we have, this is using Peng-Robinson method. Now we have to bring in the second binary analysis tool, here everything will remain same except the calculation option which will be Peng-Robinson.

So, the previous one was Lee-Kesler Plocker, this time it will be Peng-Robinson method and you run the analysis, yes, it is done. So, again we are not interested in T xy plot rather we will bring in the K values plot. So, we have to distinguish between them, so we write here binary 2, so it will be Peng-Robinson and this one is Lee-Kesler Plocker. And we have to merge the plot, so we have done and we have to use single y axis.

So, here we find that we can use only, lines no marker, fine. Here we find that the K values are almost same for the entire process except the lower portion of butane, when butane mole fraction is very, very small. Then the K values are different for whether you use Peng-Robinson method or Lee-Kesler Plocker method the K values will be different, slightly different not much. But for higher concentration of butane or heptane this difference does not exist.

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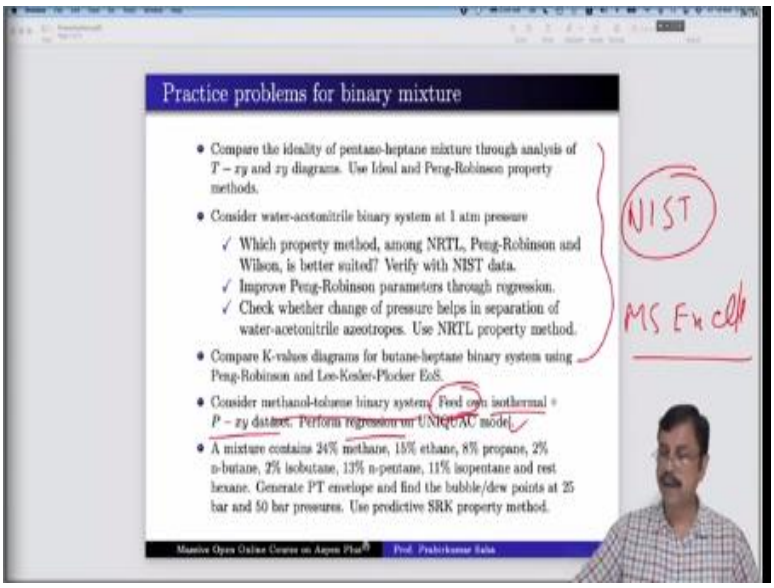

So, next problem is about methanol-toluene binary system. Now in the past we have used NIST data set, but suppose if you have your own experimental data. You might have your own experimental data in Microsoft excel sheet. So, you want to use your own experimental data for regression and some similar purpose. So, it is possible for you to feed your own data maybe it is isothermal P xy data set which we have right now in our position.

So, I will show you how to feed in some own data set and perform regression; we can take unique work model for that.

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So, let us open a new simulation, so this is methanol and toluene and we have UNIQUAC work. Now here you have to feed in your own data set, now I have the data with me in this table. Here I have an isothermal data set for P xy diagram, so this is my pressure and this is my x in methanol. So, I want to feed in this data, so let us say no, it is a mixer bring in both of them and data type it is P xy diagram.

And the temperature, so as it is P xy diagram not P TP xy, so it is expected that the temperature is fixed. So, yes, it is fixed at 31314006 Kelvin, so all of them are 31314006 Kelvin, so it is in Kelvin and 31314006. So, I have done at 40 ^{0}C, so the temperature in Kelvin is 313.14. Now we

have to feed in the data, as I have said it is P xy diagram, so it is expecting the data for pressure x and y, so this is the pressure, so just copy and paste.

So, it is simply you can use control c and control v, similarly you choose mole fraction of methanol in liquid phase control c and here ethanol in liquid phase control v. So, as soon as you write control v over here the toluene is calculated. Now at this temperature as 40 ^{0}C temperature neither methanol nor toluene will have any vapour phase. So, the vapour phase diagram will not be there. So, once this is done we can check the P xy diagram, so entire thing is my own data.

This is the experimental data that I have recorded in my own excel file that I have copied and pasted, it has not been taken from any data bank like NIST Dicamba or anywhere like that, it is our own data. So, we can press P xy and check, so this is the diagram that we have got. Pressure in bar and mole fraction of methanol against pressure, so this is the P xy diagram we have to use. Like that you can copy your excel file data onto the aspen plus domain, so you will get your own data set. And with that you can do the regression or whatever you want to do with the data you can do.

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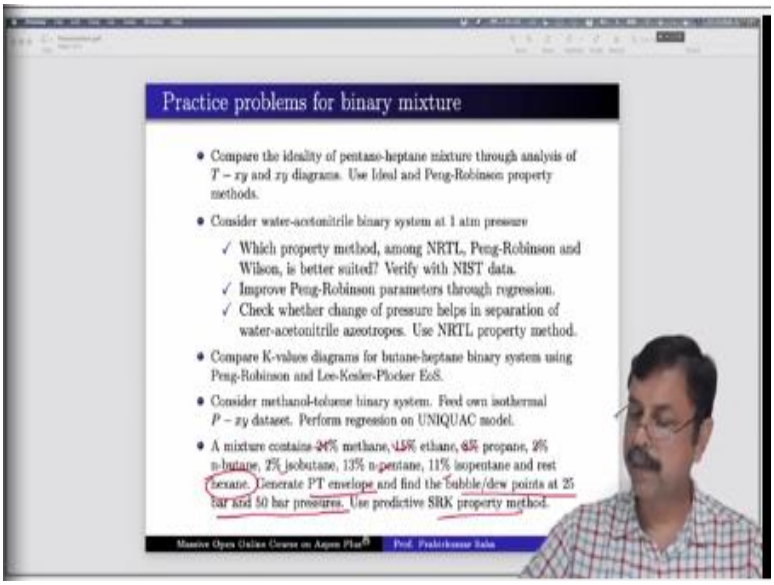

So, in the problem we are supposed to perform regression on unique work model but I leave it on to you as a task you can try it out yourself. Because you already know how to do the regression, I

have already given many examples like that. And the last problem that we have is about generating the PT envelope pressure temperature envelope for a mixture containing 24% methane, 15% ethane, 8% propane, 2% n-butane, 2% isobutene, 13% n-pentane, 11% isopentane and rest hexane.

We have to generate a PT envelope and find the bubble and dew points at 25 bar and 50 bar pressures, we have to use SRK, predictive SRK property method. So, for that let us again go to our simulation window.

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Open a new simulation and here you have to enter methane, ethane, propane, butane and then we have isobutane also. So, isobutene, we search for isobutane and we get this one and then butane, pentane and we have to find isopentane, this is the one which we are looking for 2-methyl butane and finally hexane.

So, we write it as isobutane and this one as isopentane, so press next and we have to use predictive SRK, so PSRK, run the property method. Now we have to bring in the PT envelope, this is the generate PT envelope, bring in this tool and we have to give some flow rate. So, it is in the molar percent we already have the data 24% methane, 15% ethane, 8% propane, so we can write 24, then 15, then 8 and butane 2%, 2% 13, 11 and rest is hexane. So, hexane becomes 24 + 15 + 8 + 2 + 2 + 13 + 11, so it takes total it is 75, so it remains 25, so 25 hexanes.

So, everything is set, so you can run the analysis, so this is the PT envelope that we have got. The green line is the bubble point line and blue line is the dew point line because here the temperature is higher, this is the pressure. So, we are asked to find out the bubble and dew points at 25 bar and 50 bar pressure. So, we have to check over here it is 20 bar and 50 bar, these are the 2 points, so we just bring one line over like.

So, this is the line we draw and this is another line we draw and this is the points that we are looking for. So, at 20 pressure the dew point of the mixture is 135 or 36 ^{0}C and the bubble point will be -65 to 68 ^{0}C. And at 50 bar pressure the same thing will be 175 and nearly 0 degree

maybe 1 or 2 ^{0}C respectively. So, that is how you find out the dew point and bubble point from PT envelope.

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Obviously, this entire thing will be liquid over here and this will be the vapour phase and this entire thing this is liquid plus vapour region. So, that is how we find the PT envelope.

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So, we end our problems for binary mixture, so with this we end our lecture today at this point we will continue in the next lecture, thank you.