Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 35
Bubble point method stage calculations

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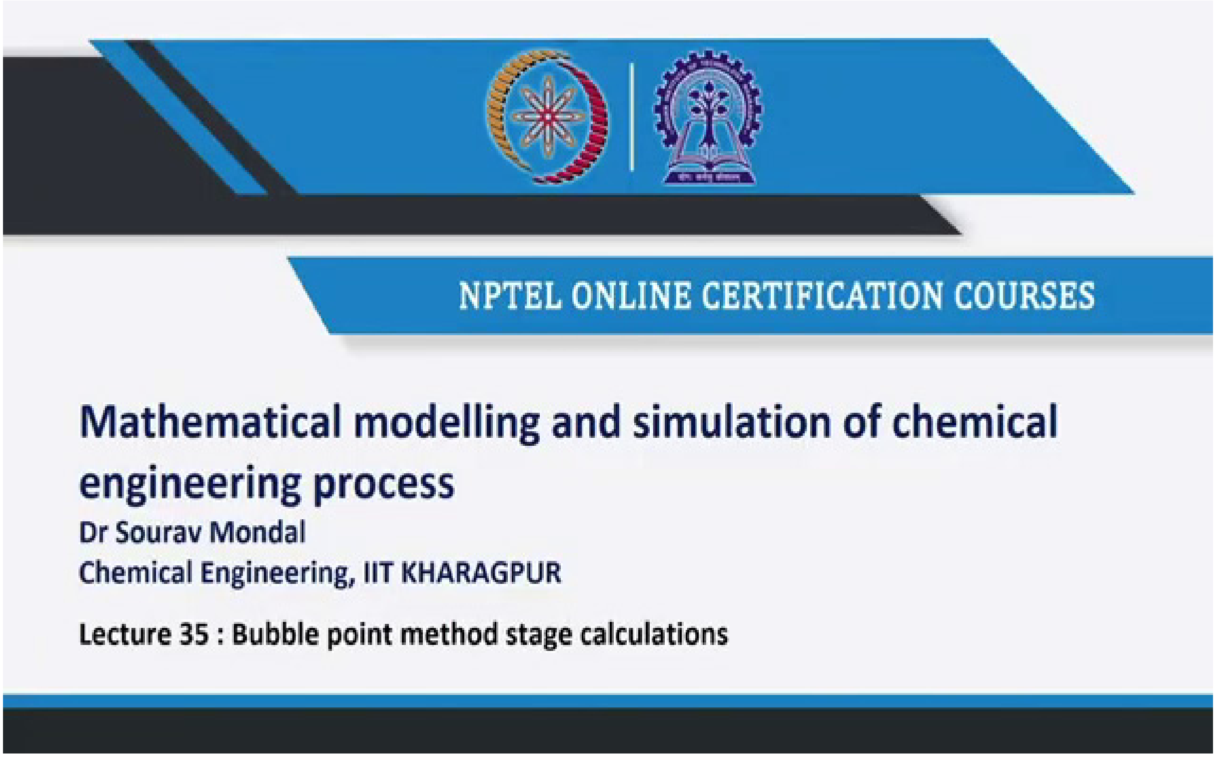

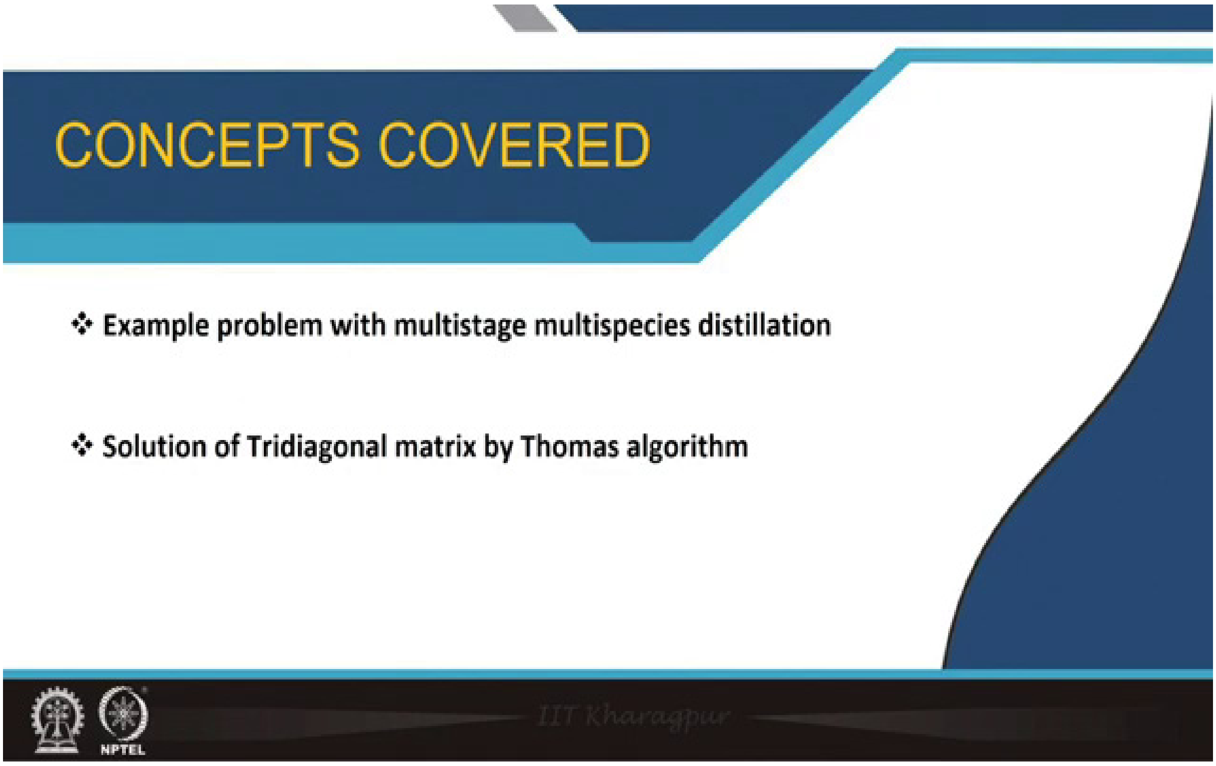

Hello everyone, in this lecture we are going to talk about an example problem related to this calculation on the bubble point method. And if you recall in the last class, we have described in detail about what are the how do you write the M E equation, how do you write the, how do you frame it into a tri-diagonal matrix.

And then what would be the algorithm of the process given that for a particular temperature or a particular this vapour flow rate you have to assume because these are the unknowns and from the degree of freedom analysis that you have to specify 1 of them for the problem to be closed. So, initially you have to guess them and then you have to proceed with the calculations and finally you have to check whether your guess values are correct or not. So, that is the idea. So, now with this idea let us look into a small simple problem and let us try to work out the first iteration step at least and in this process, we will also work out the tri-diagonal matrix using the Thomas algorithm.

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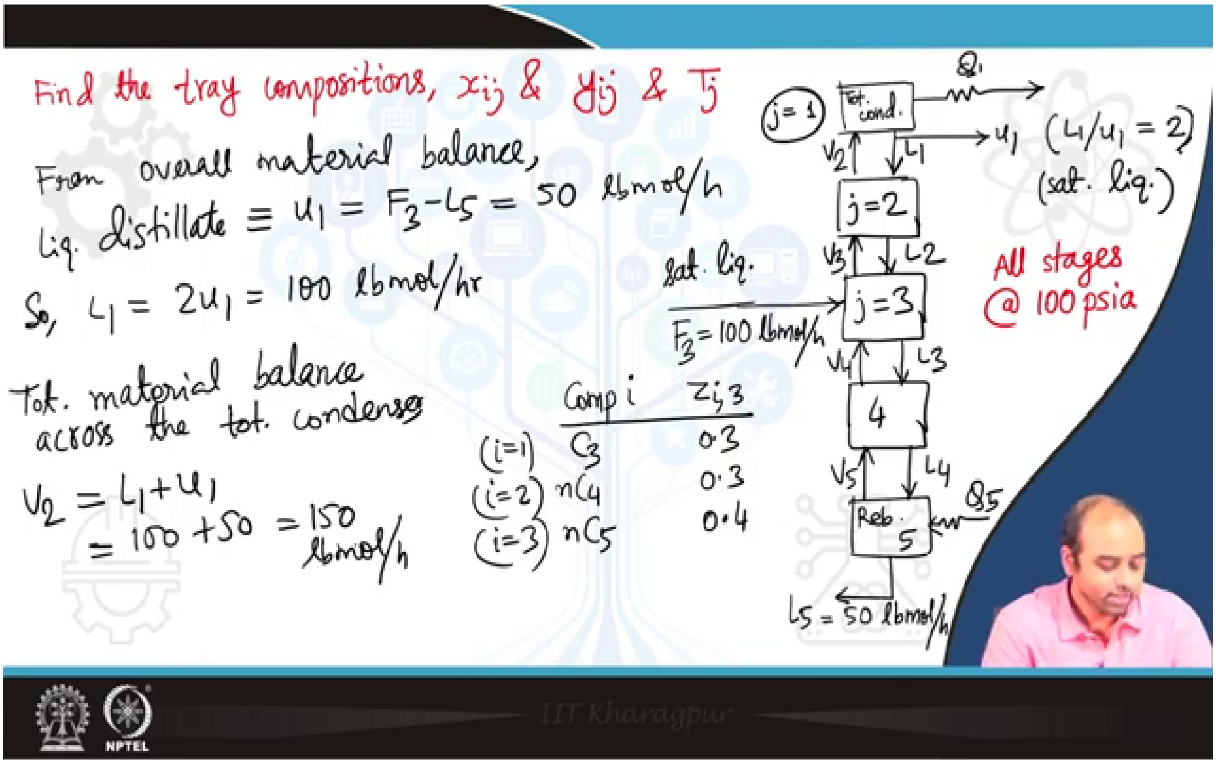

So, the problem looks something like this, let me try to draw a schematic and then try to explain you the problem. So, let us say you have this is like stage 1, you can think of and this is a total condenser is the stage 1, so let me call this as stage 1, then you have stage 2, then you have stage 3, 4 and finally you have the reboiler as stage 5, so this is reboiler which is stage 5.

So, from the top let us define these streams, so this is known as V2, this is L1 and part of this L1 is defined as u 1, as far the problem is given it is mentioned L1 by u 1 is equal to 2, this is sort of the reflux ratio condition that you can think of, and it is a saturated liquid it is mentioned as a part of the problem. Then you have this as V3 and this is L2, next is V4 L3 and this is you have V5 and L4 from the exit of the reboiler, I mean from the bottom of the reboiler you are having this L5 which is let us say is equal to 50 kilo molar pound mole per hour.

And then we are having a feed into stage 3, so let us call that F 3 is equal to 100, again this is pound mole per hour let me write it properly. So, this is, and this feed is a saturated liquid, and it has 3 components, so the 3 components are propane, butane and pentane. So, the feed compositions component i and let us write the z i 3 fractions as so this is I mean all are alkanes, so this is propane, so 30 percent, then you have n butane 30 percent and you have n pentane as 40 percent. So, this is the feed composition that you are having. There would be some amount of this Q let us say into the reboiler let us call this as Q 5.

So, all stages, all the stages operate at 100 psia, so this is the problem definition, so you have 5 stages, the top is the condenser a total condenser and the last is the reboiler. So, there are 3 physical stretches marked as j is equal to 2, 3 and 4. And then you have a feed saturated feed into the system and the composition etc., are known all the feed compositions is known and all the stages are said to be operating at 100 psi or the constant pressure and the product that you are taking down from the reboiler is also given that is 50 kilo molar pound mole whatever the some units is there and the feed that you are getting is 100 pound mole per hour, L 1 by u 1 that ratio is given as 2. So, essentially that relates to the reflux ratio of the problem.

So, now the task is to find out the temperatures as well as the tray compositions, so please note that this is not a binary system anymore, you have 3 components and 5 stages we have to calculate what are the tray compositions as well as the temperatures. So, this is the objective. So, find the tray compositions x i j and y i j, so this is the important part of the problem and of course as well as you have to also find out the Tj the temperature of each of the tray.

So, since this composition this alkane, then you have I mean among the alkanes you have propane, butane and pentane, so naturally propane would be the more volatile components you would expect more propane on the top, so C 3 would be more on the top and C 5 would be more at the bottom. So, this is i is equal to 1 this is i is equal to 2 and this is i is equal to 3 and here everything is in terms of j, so this is j is equal to 1, this is j is equal to 2, this is j is equal to 3 so on.

So, now I mean before we go ahead with the bubble point calculation, the first thing to work out is just work out some quick mass balance and try to get as many streams I mean knowledge of as many strings as possible. So, from overall material balance what we get? So, from the overall material balance, we get that the liquid distillate that is u1 is equal to F 3 minus L 5, this has to balance the total mass has to balance, so only you are taking out is u 1 and L 5 and entering is F 3. So, if you put in the numbers this turns out to be 50, 50-pound mole per hour, easily you can get that. And also, it is mentioned that L 1 by u 1 is equal to 2, so L 1 is equal to 2 u 1, which is equal to 100. So, these are some straight calculations we can do.

If you do a total balance, total this mole balance, sorry material balance let us talk it in general terms total material balance across the total condenser what you get, this V2 is equal to L1 plus u1, across total condenser again mass balance has to be satisfied. So, which is equal to 100 plus 50 you have so this is 150-pound mole per hour. So, these are some of the streams which we can easily calculate it out from the knowledge of the mass balance.

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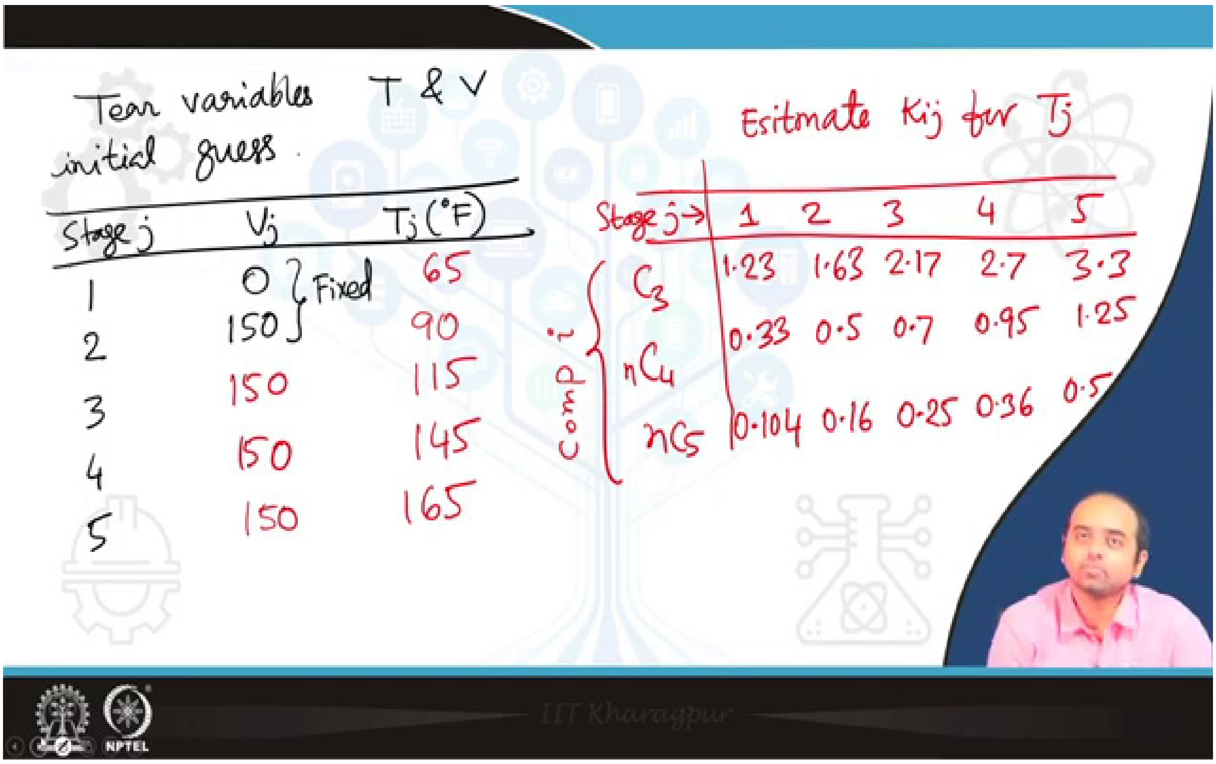

So, let us consider the rest of the V is not known so like V 3, V 4, V 5 are not known, because the other liquid flow rates are not known. So, the tear variables in this case, in this problem are T and V, that is only not known, so we have to make an initial guess. So, we have to make an initial guess for this T and V across different stages, this is the problem is in British unit guess in terms of Fahrenheit.

So, stage 1, 2, 3, 4, 5, so V j at stage 1 I mean this this 0, there is no V j value, so stage 1 we put it as 0, from stage 2 we get 150, so these remember these 2 are fixed by the calculation they are not guessed. So, for the remaining stages the first logical case would be consider them all equal.

So, for the remaining stages, let us consider them as all equal, as far as the temperature is concerned, as far as the temperature is concerned, I mean how do you make a guess I mean you cannot take some arbitrary value I mean of course guess is an arbitrary value. So, generally we know that at the stage 1 you are expected to get more of the, this propane and at stage 5 you are expected to get more of the pentane.

So, the dew point of propane is what would be the condenser temperature and similarly the dew point of pentane would be the temperature of the bottom. So, accordingly we can make a guess, it may not be accurately at that value but this is like 65 and this is typically 165 in terms of Fahrenheit, so this is roughly the boiling point of this pentane at 100 psia.

And similarly, the boiling point of pentane at stage 5, which is like you are getting the more enriched product is the pentane, because that is the heavier component among these three, so that is the boiling point of pentane and 65 is more or less the boiling point of this propane of course it will be a mixture it will not be pure propane, but at least for the guess these are the values we can take. And remaining values we can make just a quick linear interpolation, difference of something like 25 degrees across each tray.

So, these are the guess values, so these are the guess values or the estimated values that is something we can start with. So, now the immediate thing that we should do once we calculate this temperature is to estimate this k i j, estimate once this guess values of the temperature you know some information on the temperature, the next part of the calculation is to guess or to estimate the k i j, so you do not guess the k i j you estimate k i j for the known values or whatever the guess values of T i j.

So, k i j values would be different for the components and then it will be also dependent on the temperature. So, let us say we write the stage j here, so that is 1, 2, 3, 4, 5 and the components i here C 4, C 5, so this is like the component i. So, if you look into some of the lookup tables to calculate these values you can estimate out how k i j can be worked out and also you can also use some other formula or something whatever and these values you can typically also obtain from any property handbook.

So, let me write down the values and you will see that the k values increase as temperature increases that is what you see that along the row it increases and k value decreases as the molecule becomes more heavier that is what we see that as you are talking about higher carbon number the k value decreases. So, these are the k values. So, once you have knowledge of your k values then the next step is to start trying to form the tri-diagonal matrix. So, let us move forward in that direction and try to estimate the different coefficients.

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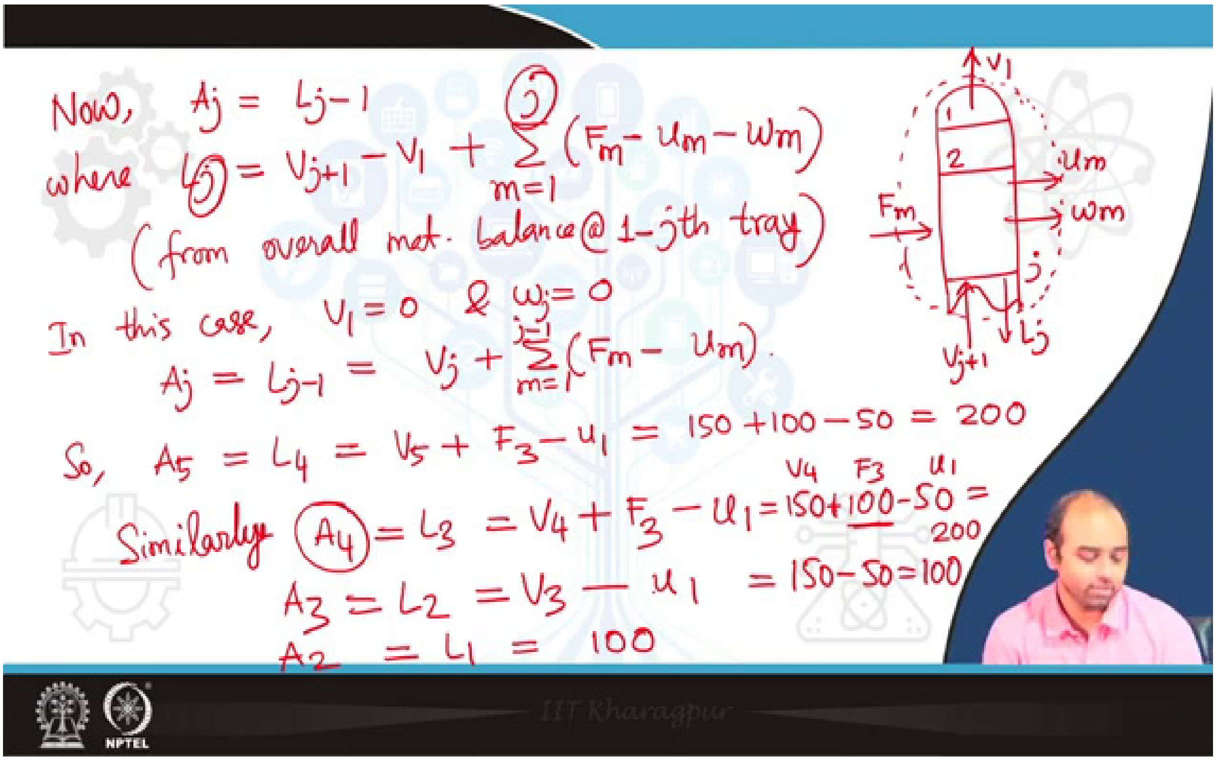

So, this is the simple schematic of the distillation column, this I am just writing it down for your help and for better visualization of the picture. So, let us say this is V1 even though there is no V1, but let us write it down in that way, so we can work out some more mass balance, this is a generalized picture.

So, now what we have we will refer to the generalized pictures, A j, so that is the A coefficients in a tri-diagonal matrix is equal to L j minus 1 and what is this L j? So, if you try to take this picture across any jth tray L j, L j is something which is coming out of the system and that is equal to the amount that is taken out from the system as well as if you do a mass balance across any jth tray, I mean the mass balance considering the rest of the column across j tray. So, L j would be V j plus 1 that is introduced into the system.

Then minus V 1 because V 1 is leaving the system plus this amount of F m minus u m minus W m, so there could be any possible values of this F, so F can be I mean this j can be within the feed stem in the jet number can be within the feed tray without the I mean it could be before the feed tray whatever, so this is like the generalized form. So, L j is V j plus 1 minus V 1 that is what is leaving from the top and plus of the remaining whatever this field it is introduced side cuts that you are having u m, w m across any tray, so whichever tray does not have this u or w will be equal to 0.

So, this is actually from the overall, so from the overall material balance at jth tray, so it is not only across the jth tray but from 1 to jth tray. So, it is like 1 to jth tray. So, now using this idea I mean in this case, if we put in the numbers, we know that V 1 is equal to 0 and there is no w, so w is equal to 0 for any tray, so w j is equal to 0 for all the trays.

So, for the first one I mean if I try to write A j which is equal to L j minus 1, which is equal to V j V I mean V 1 is again 0 plus I am having this m is equal to 1 j minus 1, because that is for L j, so it is the this subscript j is for L j, now if it is for j minus 1 it will go up to j minus 1 this summation we just follow the index pattern now F m minus u m.

So, what about A 5? A 5 is equal to L 4 and which is equal to V 5 plus other than F 3 there is there is no other F, F1, F2, F3, for everything is 0 and minus u 1. So, you already know what is your V 5 in the system, because we already have all the V information from the guess values, so V 5 is 150 plus 100, F 3 is given 100 and u 1 is also mentioned as 50. So, this turns out to be 200.

So, similarly you can also do A 4, A 4 is equal to L 3 and this is equal to V 4 plus we have F2 minus u 1, now we know F 2 is equal to 0. So, V 4 is 150 all the V are 150 and u 1 is u 1 is how much 50, so this is equal to 100, sorry this will lead to L 3 is equal to F 3, so this is not F 2 no L 3 will lead to F 2 that is right and F 2 is equal to 0 and therefore you are going to get and you are having u1 yes, so it is 150 minus 50 is equal to 100 that is A 4, A3 similarly you can also work out your A3 and A3 is equal to L 2, which is equal to if you put in the values that is V 3 plus F 1 minus u 1, so this is once again 150 minus 50 this is equal to 100.

Similarly, A 2 you can also work out that is equal to L1 and this is also 100. So, guys there is one small correction here, so in in while calculating this A 4 you will see that we are doing it V 4 plus I mean F 3 like F 3 plus F 2 plus F 1 but F 2, F 1 all are 0, but F 3 is only non 0 that is why I have written down only F 3 and minus 1 because u 2, u 3 are also 0, so this gives you 150 plus 100 that is so this is V 4 and this is your F 3, so this is V 4 F 3 and this is u1, so that gives you 200. Similarly, you can also work out A3, A 3 is only V 3 minus u1, because there is no u2 and there is also F 1, F 2 both are 0, its only F 3 that only exists. Similarly, A 2 is equal to L 1 and you can put in again the numbers that is V 2 minus u 1 that is you will give you 100.

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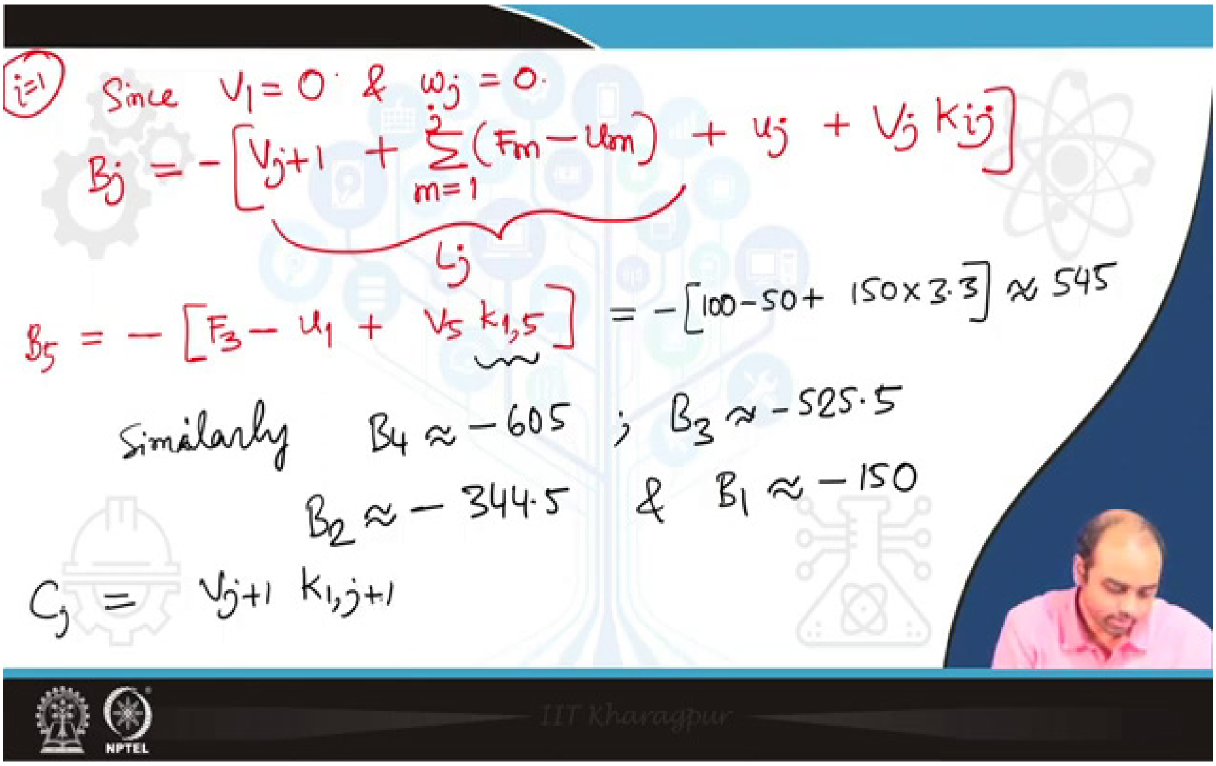

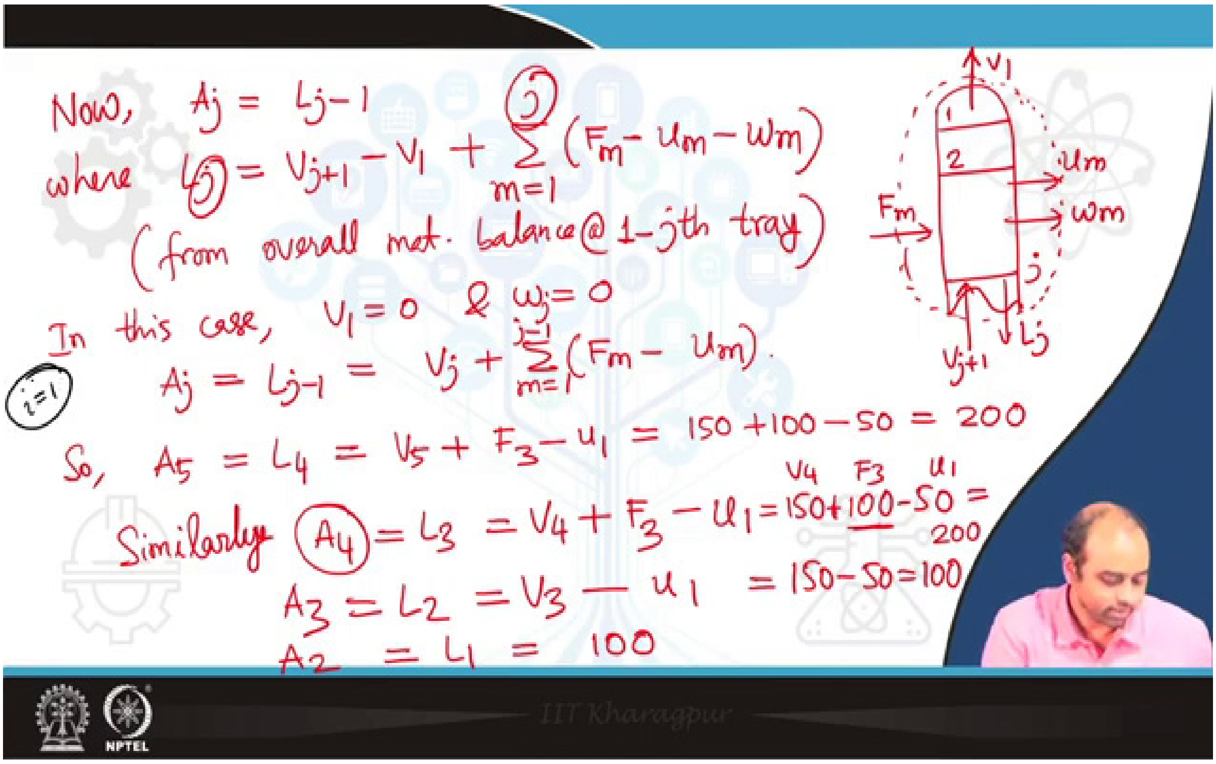

So, again we can write down next about the B terms, so since V 1 is equal to (I mean) sorry 0 and w j is equal to 0, we can write for B j, V j plus 1 plus summation of everything is minus so if you recall this B j, this B j is, I mean it does consist of the L j term, so this is nothing but your L j, L j plus u j plus V j and w j is 0 that is why I have not written down this w j from the last class if you recall that is L j plus u j plus V j plus w j together k i j. So, this component L j I am written down from the mass balance as V j plus 1 summation of this quantity and of course w is equal to 0 that is why I have excluded the w.

So, now with this idea we try to calculate what do we get for B 5, so B 5 is F 3 minus u 1 plus V 5 into k 1 comma 5. So, this all we are at the moment we are all trying to do for i is equal to 1, let me just say this, this all whatever this A values I am writing it down this everything is for the case of i is equal to 1. So, this is what is B 5.

And so, if I put in the numbers, if I put in the numbers of k I mean this k and everything F 3, u 1 we know there is no V 6, V 6 does not exist in this system, so that is equal to 0 so it is only F 3 minus u 1 and V 5. So, if you put in the numbers you are going to get, so approximately this will give you 545-pound moles per hour. Similarly, you can also write B 4 as minus 605, then B 3 also you can write minus 5 to 25.5, B 2 you will also be getting 344.5 and B1 is minus 150. What about C j? So, C j is equal to V j plus 1 into k 1 j plus 1.

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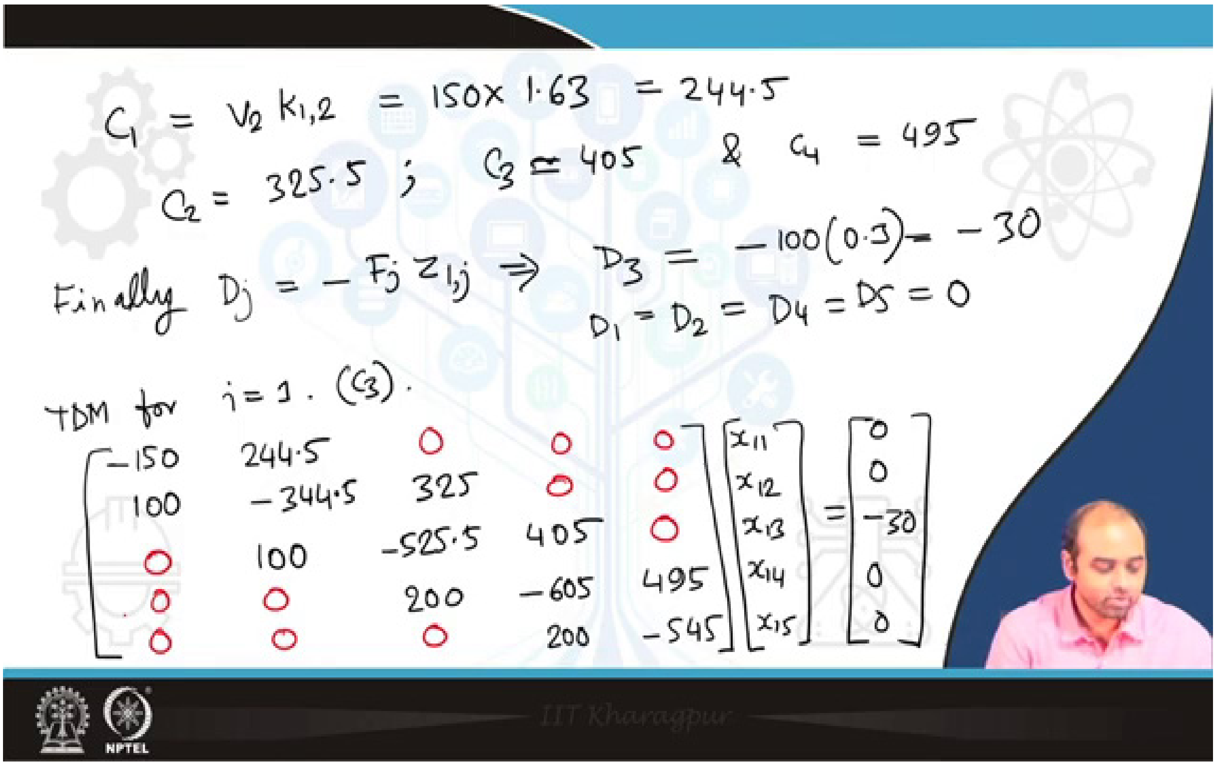

So, C 1 is equal to V 2 k 1 comma 2, so it is equal to 150 into 1.63 that is V k 1 comma I mean 1 2 that is the value of the equilibrium constant at stage 2 for propane. So, similarly you can also get C 2 I am just writing it down here and it is something you should cross check it out yourself. Please note that there is no C 5 in the system in the tri-diagonal matrix if you recall the last row I mean does not have this C 5, similarly the first row does not have the A1 component.

And finally, we have the D, so D j which is the right-hand side vector is equal to minus F j z 1 comma j, so as you can realize for this only D 3 will exist. So, that is minus 30 and all the rest of the D that is D 1 you are having D 2, D 4, D 5 all are equal to 0. Now, how do you get the TDM, the tri-diagonal matrix, TDM for i is equal to 1 that is for C 3, so we try to fill up the matrix.

So, first there is no A 1, it starts from B 1 and B 1 is already we have noted down minus 150 and C 1 is 244.5, then you have A 2, B 2, C 2, then we have this A 3, B 3, C 3, then we have A 4, B 4, C 4 and finally we have A 5 and B 5, so please note that all the B components are negative and here you have x 11, this is x 12, x 13, x 14, x 15.

And on the right-hand side you are having 0, 0 minus 30 and also 0, 0. So, in the tri-diagonal matrix as you can see these are the only terms the rest of the term are essentially 0. So, this is a 5 by 5 matrix depending on how many number of stages you are having in the system will determine what is the size of this coefficient matrix.

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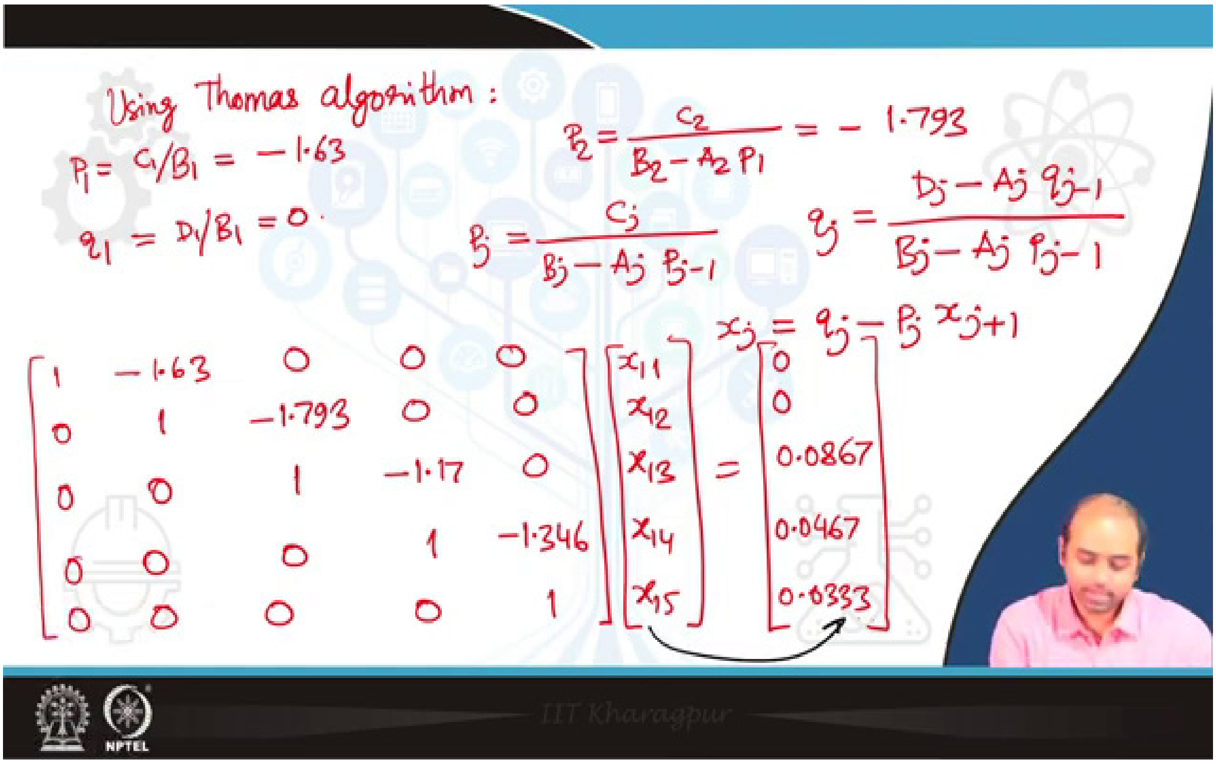

So, we will use the Thomas algorithm here to calculate out the this value, so using Thomas algorithm what do we get P1 is equal to C 1 by B 1, so if I put in the numbers I get minus 1.63, similarly P 2 is equal to C 2 by sorry B 2 minus A 2 P 1, this is equal to 1 minus 1.793, so and q 1 that you see is D 1 by B1 that is equal to 0. So, like this if you proceed and try to calculate the rest of the P and the q j values, I hope all of you recall the formula of this P and j.

So, the generalized P j can be written down as C j by B j minus A j P j minus 1 and similarly the q j formula is D j minus A j q j minus 1 this is a recursive formula, B j A j P j minus 1. So, the idea is that we have x j is equal to q j minus P j into x j plus 1. So, essentially, we are going to transform this tri-diagonal matrix with only the diagonal elements as 1 and essentially all the A parts will be going to 0 and we will be having only the C terms as our q j sorry P j terms.

So, the tri-diagonal element I mean the tri-diagonal matrix will look something like 1, then you are having minus 1.63, so 0 1 minus 1.793, then 0 0 1 and then you are having minus 1.17 and finite is 0, 0, 0, 0 and 1, remaining are 0 elements. So, and here you have x 11, x 12, x 13 and on the right-hand side you also have this matrix, so this is 0 0 then you have so this you can clearly see that the last one can be easily said to be at 0.033.

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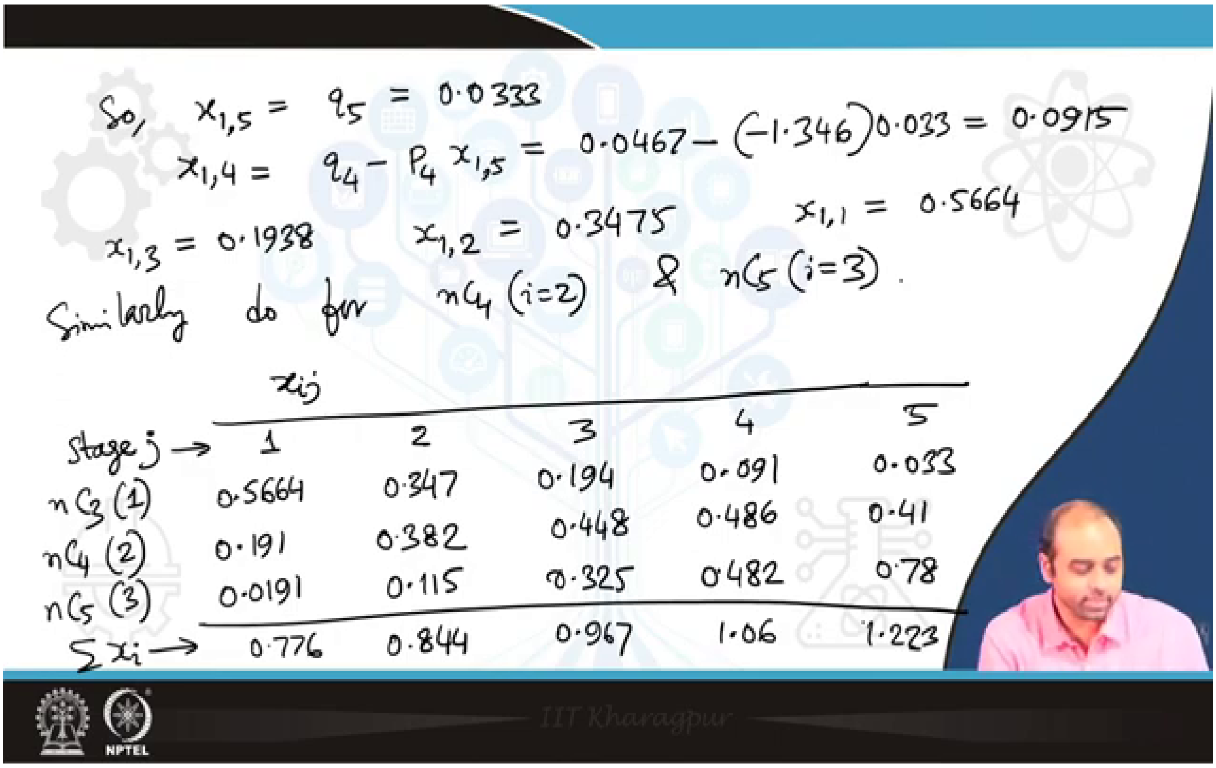

So, x 1 comma 5 is nothing but q 5 in this tri-diagonal matrix which is 0.0333, similarly x 1, 4 can be written down as q 4 minus P 4 x 1 comma 5, so this is 0.0467 minus 1.346, I am just writing down the whole numbers, so that this the calculations become very explicitly understood.

Similarly, you can also do x 1 3, so that will give you 01938, x 1 2 you can easily realize that as we are moving towards the top this propane concentration of the fraction increases. So, now if you so similarly you can do for similarly do for nC4 that is i equal to 2 and nC5 these you can work it out yourself.

So, now let us look into the x i j matrix, let us work this way let us write down the stage j as 1, 2, 3, 4, 5 and this is nC3, so we write down the values. So, you can see that as we go down the propane concentration decreases for nC4. Similarly, this is for i is equal to 1, this is for i is equal to 2, if you work it out you will see so as we move down the heavier components becomes more enriched. Similarly, I can also write nC5, for each case you have to work out the tri-diagonal matrix and get these values.

So, you can note that the heavier component is less in the top tray and it is more at the bottom tray, so the important thing to do is to do have the summation of x i's, so this is across i this summation needs to be done across all the stage and if you see that this summation does not come to 1, because we started with the guess value and it is primary for this purpose that this needs to be normalized. So, in one of, I think in step 3 or step 4, we said that it is necessary to normalize the individual tray compositions.

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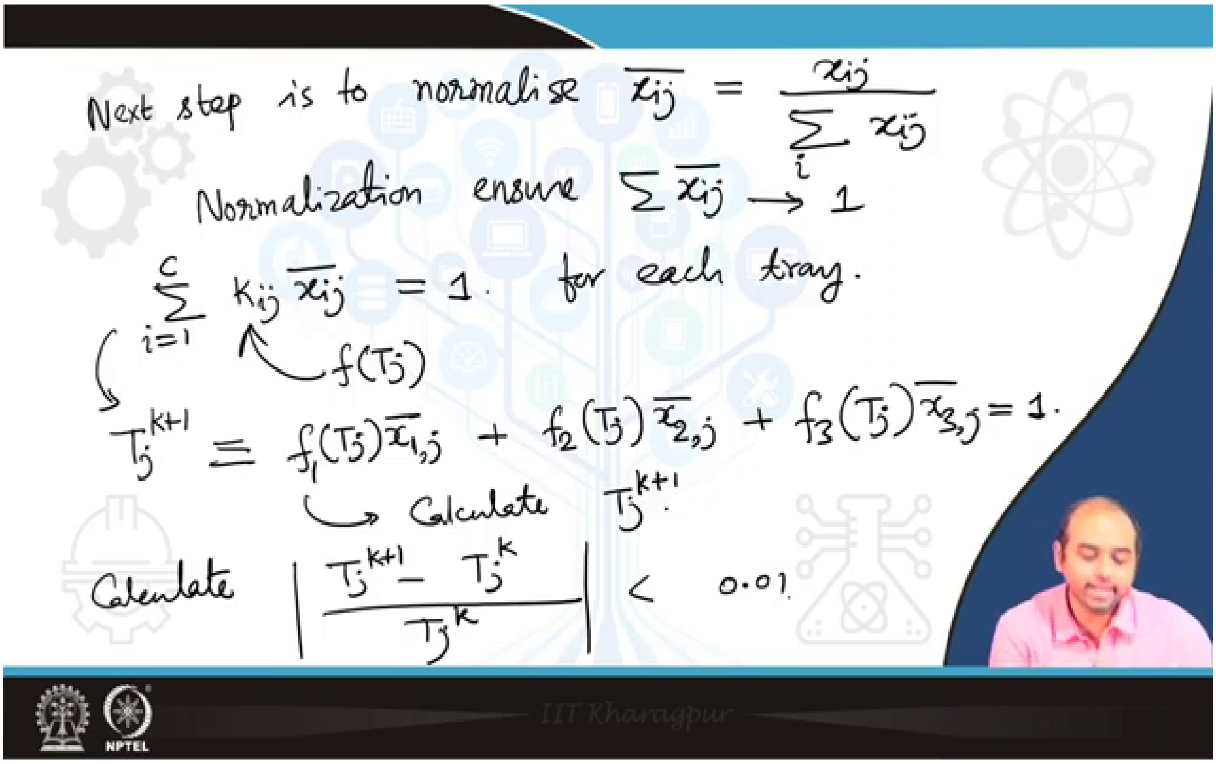

So, next step you need to do is normalization, let us write the normalized as bar, so that is x i j summation of over i’s at each tray. So, once you do this then these fractions would be changed or would be modified. So, normalization will ensure, so this normalization will ensure that the summation of the normalized tray composition is equal to 1.

So, similarly now use the other one that this one to be equal to 1 for i is equal to 1 to C and this you do it for all the stages this for each tray this needs to be satisfied. So, from there you back calculate out what is your T j, because this k i j is a function of T j, to satisfy this equation then you work out what is your T j.

And then you determine whether this T j that you are getting in this iteration I mean it is something that you can also work out. So, what it will look I mean the equation what it will look if you just convert it here for the equation of T j, you will some function of T j, then you are going to have x 1 j plus F 2, so this is F 1, this is F 2 j, then you are having x 2 j. So, this summation will actually convert like this F 3 individual functions.

So, from this equation you calculate out calculate T j and then match that this T j whatever you are getting here how much it is different from the initial guess. So, calculate this relative error that T j whatever you got now how much it is different from the previous one, the guess one and let us see if this ratio, it is always good to have this in absolute quantities, if this ratio is a tolerance let us say 0.01 or 0.001, this relative ratio then it is acceptable this temperature is acceptable, then you go on to find your V j and do the same I mean once your T j, then you can use the enthalpy balance relation.

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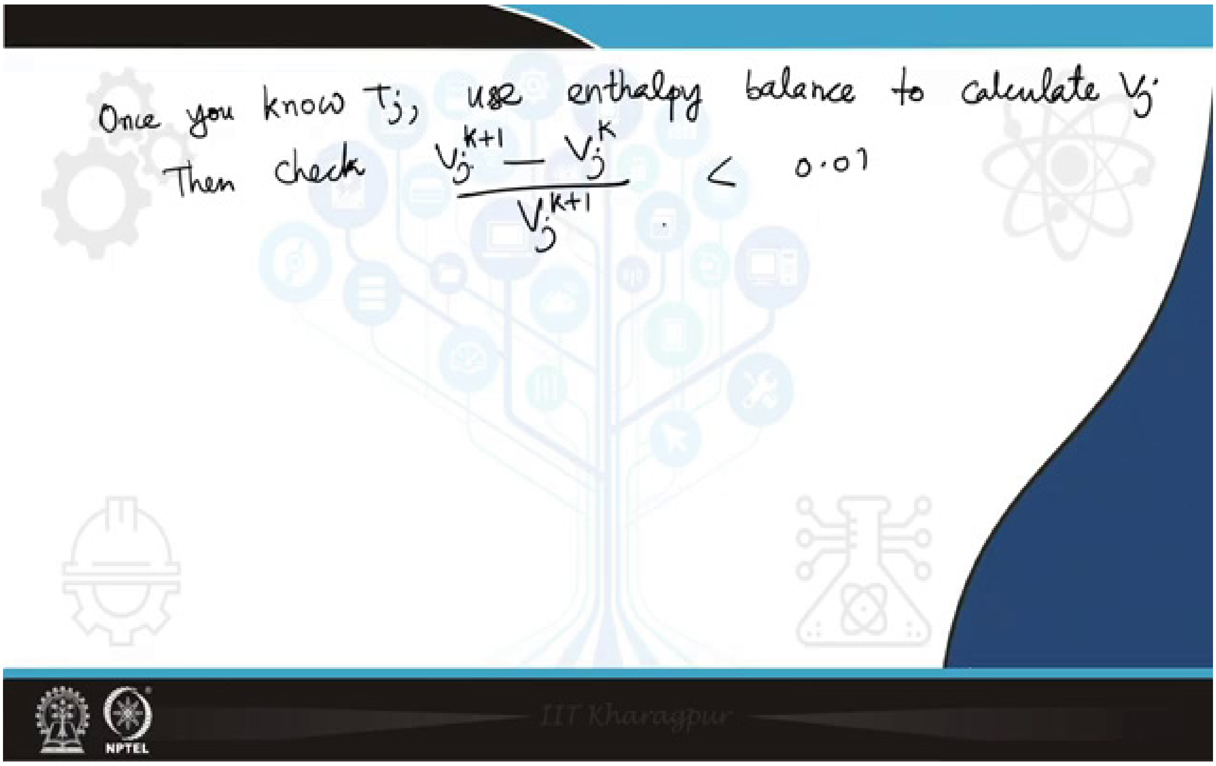

So, once you know T j use enthalpy balance to calculate V j and then check whether the V j that you got now in this after the end of the calculation is how much it is different from the starting guess, if this satisfies then it is fine your calculation is converge, if not then you consider your new guess as this V j whatever you got now.

So, that is how this calculation needs to be done in an iterative way every time you have to solve the tri-diagonal matrix for each of the components. And then finally you calculate out normalize them calculate out your T j and from there you can estimate what is your V j from the enthalpy equation.

So, I hope all of you understood the background of this calculation steps and this is very essential because you unless the nitty-gritty of the calculations you cannot be confident about what kind of solutions you are getting from whatever let us say you use a proper simulator or you develop your own code what should be the reasonable choice of the initial guess and everything will not be known to you, how does the TDM calculations affect in the computational resources and everything.

So, I hope all of you found this lecture to be quite interesting and useful I also encourage all of you to do yourself an exercise problem or a similar type of problem or maybe this problem itself you try to evaluate out for the next iteration and see whether the temperature and everything you are getting convergence or not and that will give you more confidence on the calculation steps. Thank you I hope all of you liked the lecture.