Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 34
Tearing method

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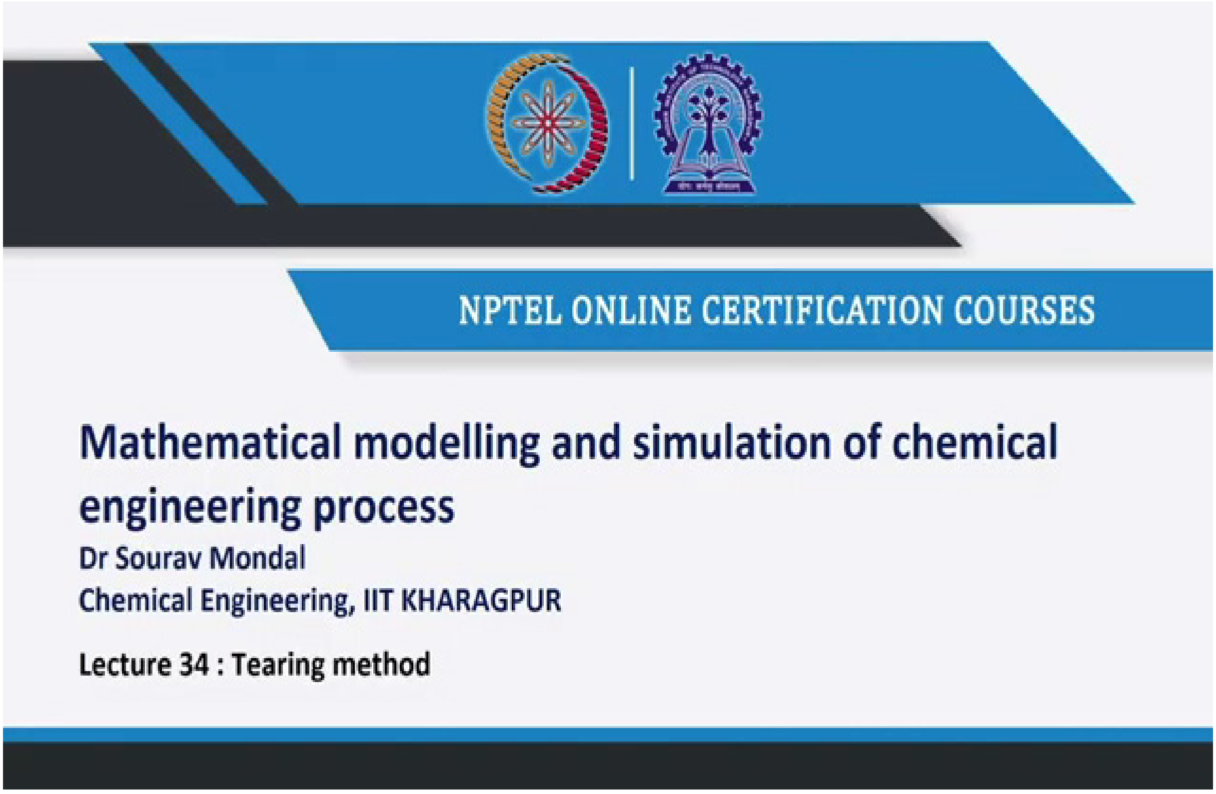

Hello everyone, so in this class today we are going to talk about the Tearing method, essentially the bubble point calculation method and we will talk about its algorithm and in the next class we will solve one example problem.

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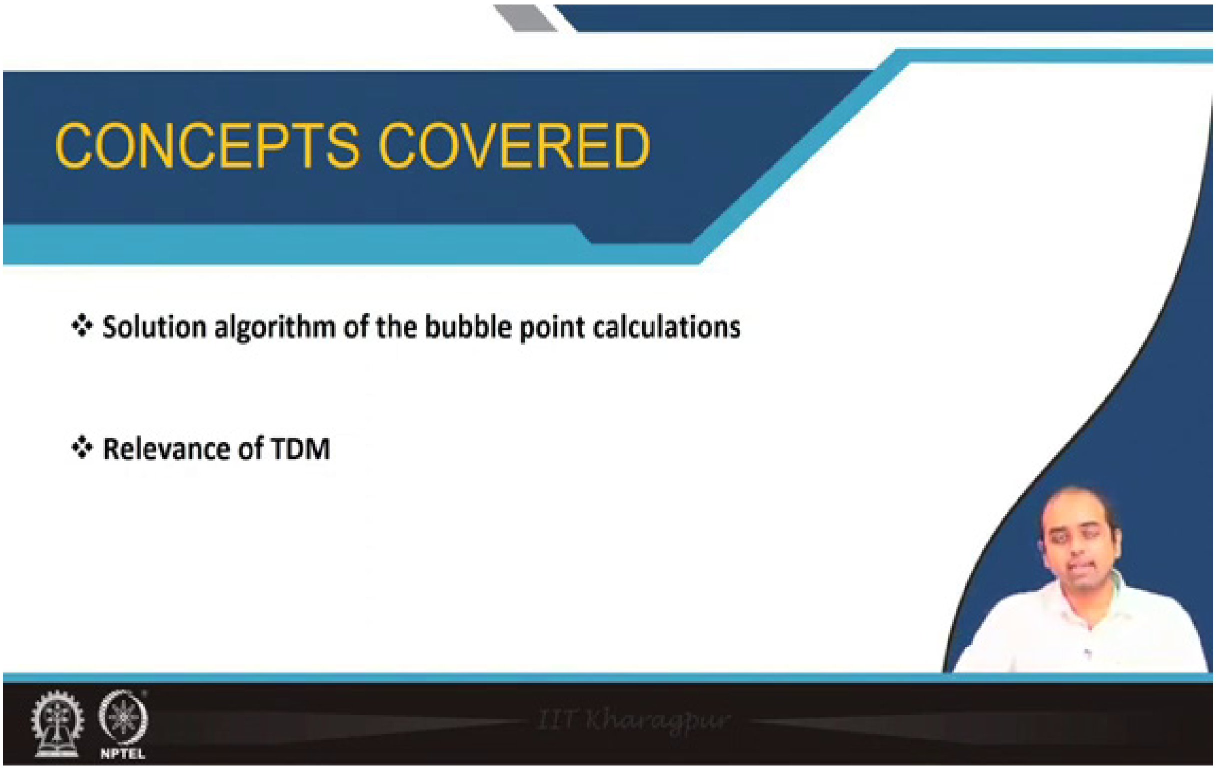

So, unless we talk about example problem, things are not so well understood. So, here we are going to talk about the bubble point calculations and the process of obtaining or the necessary equation framework and how you arrive at the tri diagonal matrix formulation in this case is something which I want to highlight.

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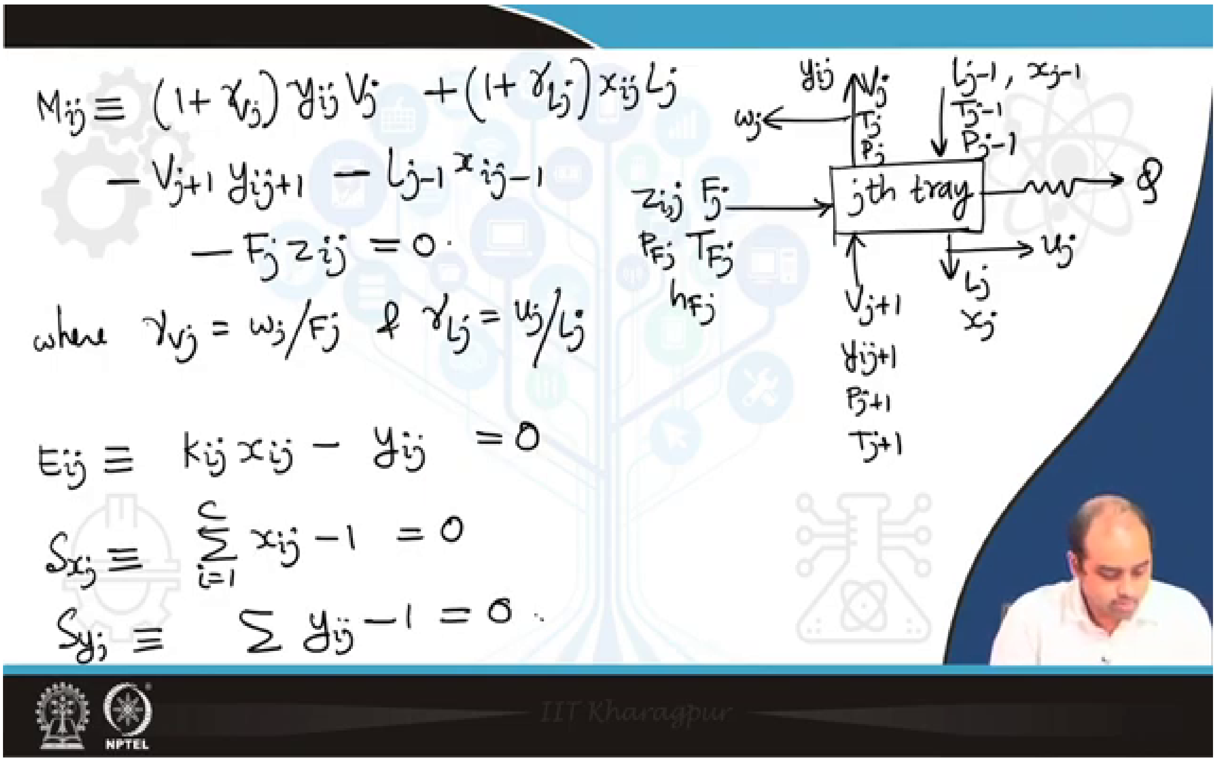

So, before as we start first, let us write down the mesh equations, so I will just quickly try to draw the tray just for the sake of clarity and for the sake of understanding. So, let us say this is my jth tray, so I have this is v j, this is sorry I should not write like this, I should write like this v j plus 1, this is L j, this is L j minus 1, you have a side cut we have defined this as w j side cut here is denoted as u ,j the heat component is Q and there is the inlet feed Fj, you write down the this y i j, this is y i j plus 1, this is x j and here where x j minus 1 and here we are having z i j.

So, similarly you have T j, P j and you have P j plus 1, T j plus 1, you have T, I mean liquid and vapour strings need not to be written down. Here you have T j minus 1 and you have P j minus 1. These are generally the specifications of course L and the enthalpies are also written down as h P j and h L j, I am also writing down the temperature and the pressure of the feed stages.

So, the M equation the c number of M equation, this is just a recap from the last class, so we will just go through this quickly. So, this is the vapour, that is into the system plus liquid that is into the system minus vapour, sorry this is vapour leaving the system minus the vapour that is introduced to the system and minus of the liquid that is introduced into the system and minus the feed that is introduced into the system, where gamma v j is the fraction of the side cuts, this close not to avoid any confusion. So, this is the M mesh equations. Then we have the E equation so E i j is written down as k i j x i j minus y i j equal to 0, you also have the summation equations, both for the liquid component and for the vapour component.

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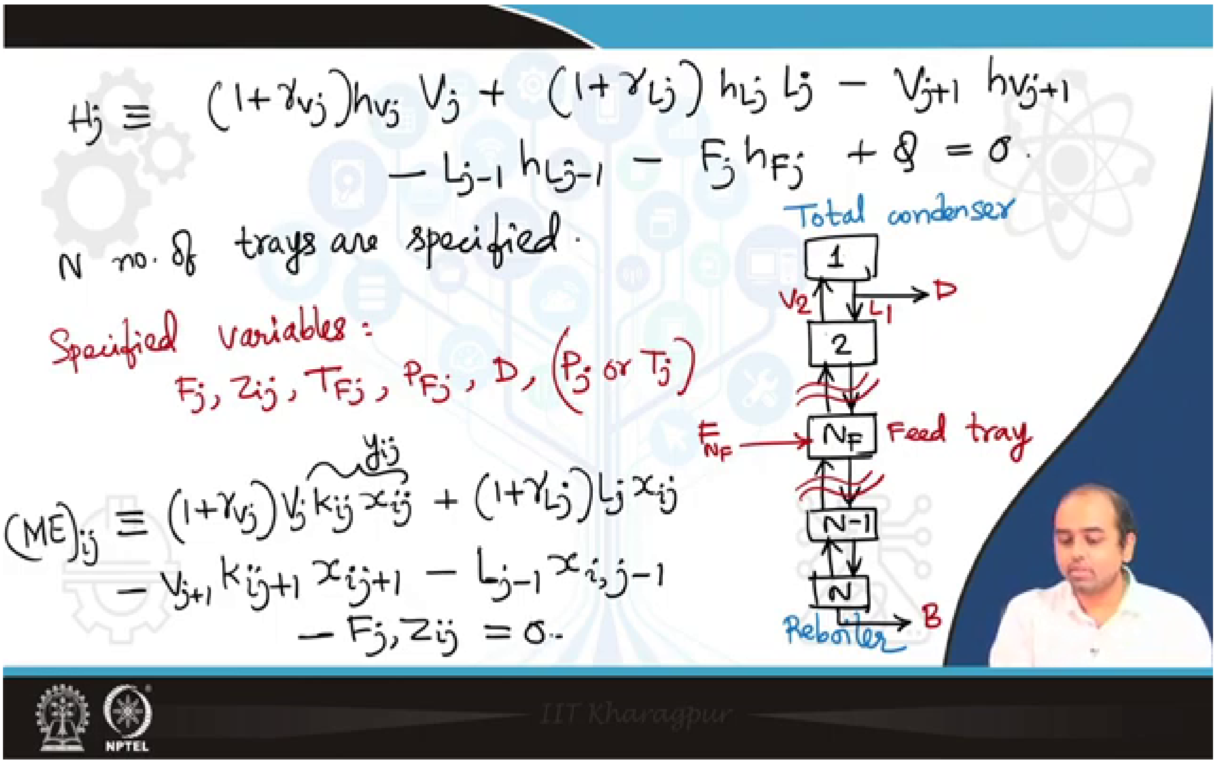

Next, we write down the energy equation also. So, this is the energy that is going out or the enthalpy leaving the system, in the form of vapour and in the form of liquid, this is the vapour entering the system and this is the enthalpy of the liquid entering the system and this is the enthalpy of the feed stream and here is external heat. Now, let us see that if N number of stages in N number of trays are specified, let us say you have the tray nomenclature as like this. So, I mark this one as the total the top one has total condenser and the bottom one as Reboiler.

So, the let us draw the streamlines here, stream connections like that here, so this one is V2, this one is L1, please note the subscript, this is the side cut D, this is a feed tray. So, there will be some intermediate stages like till from 2, it is not like 1 2 and then n f, similarly here also there are some intermediate stages which is not shown here. So, the feed to the feed tray is F, F NF you can also write something like this and the reboiler is B, I mean the B is the side cut or the flow rate from the reboiler.

So, from here the specified variables for this case are of course the number of stages that is known, then you have F j of course number of stages does not come in the part, F j then we have z i j, T F j, then you have P F j, then you have D in the problem, then B is also specified rather B is something that you can also calculate out from the overall mass balance.

And let us say the pressure in the system is specified for P j for all the stage either pressure or temperature, whatever one of them either pressure or temperature is specified for all the stages. So, now from the now let us work out the equations and if you try to form the generalized equation you will you can relate each of these coefficients in the material balance, the heat equations together.

So, what we are going to do? I am going to write down the material balance and the maybe I can write it down here the equation together M E equation together. So, what I get I want to remove all the x i j's, sorry all the y i j's into x j's. So, this is v j, then I have from the equilibrium relation as k i j, x i j, so this part is nothing but your y i j before and plus you have 1 plus gamma L j, L j, x i j, then we have minus of v j plus 1, k i j plus 1, x i j plus 1, minus L j minus 1, x i j minus 1, minus F j z i j is equal to 0. This is the M E i j equation I can write it down.

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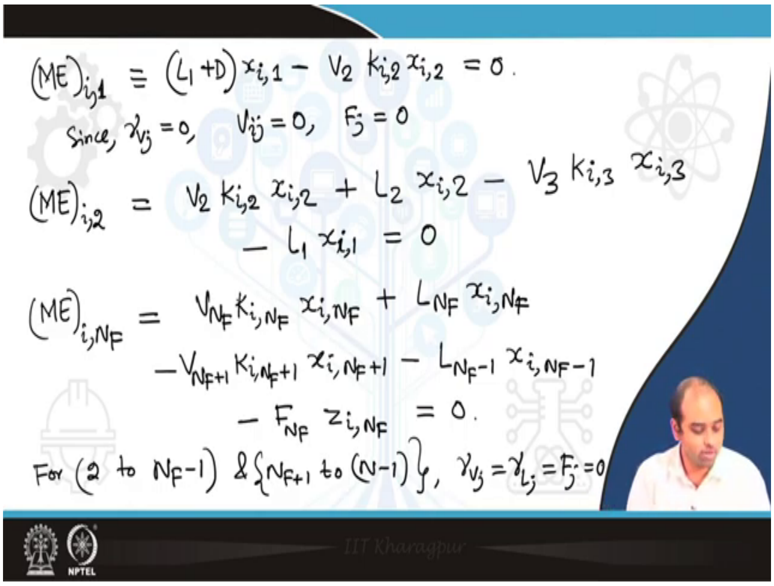

Now, let us look into how what how does it turn out for the first stage. So, M E, i comma 1 will be L 1 plus d, as x i 1 minus V 2, k i 2 x y 2 and rest are 0, because gamma V j is equal to 0, V i j for stage 1 is equal to 0, F j is equal to 0. Similarly, M E i comma 2 can be written down as V 2 k i 2 x i 2 plus L 2 x i comma 2, minus V 3 k i 3 comma x i 3 minus L i x i comma 1 is equal to 0. So, all the vapour and the liquid flow rates are there is no side cut and of course there is no feed tray.

Similarly, for the I am only writing some of the k some of the important ones and the rest would be all similar M 2 would be similar to M 3 and M 4 etc except for the feed stage. So, V

N F k i N F, then you have x i N F plus, so all this would be same, L NF x i NF minus V NF plus 1 k i NF plus 1 x i NF plus 1 minus L NF minus 1 x i comma NF minus 1.

And then we have the feed that is F NF, which is nothing but the feed z i comma NF, this would be equal to 0. So, from 2, so ideally what we get for 2, to NF minus 1, we have so from 2 to NF minus 1 and NF plus 1 through almost the stage before the reboiler, for all these parts you have gamma V j, gamma L j and F j all are 0, these parts does not come in the picture generally unless you have some specific multiple fields and all are different side cuts and all, generally this is this is not this does not exist.

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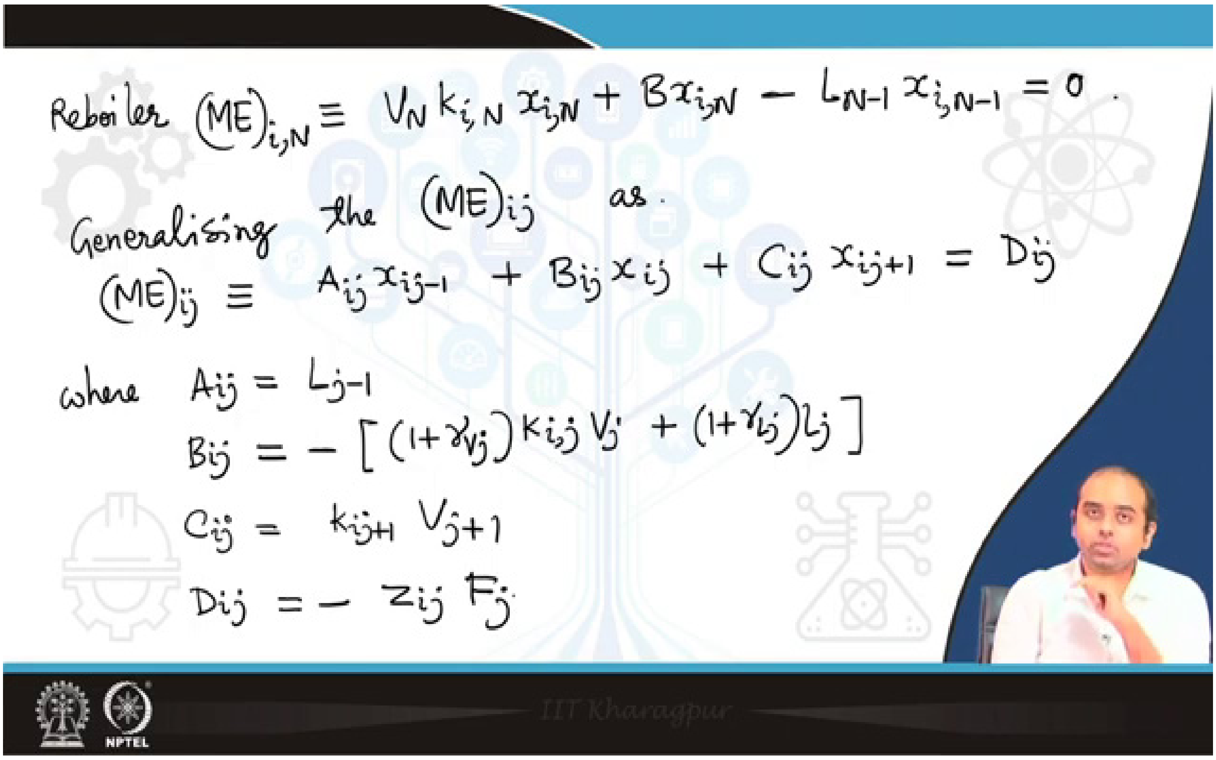

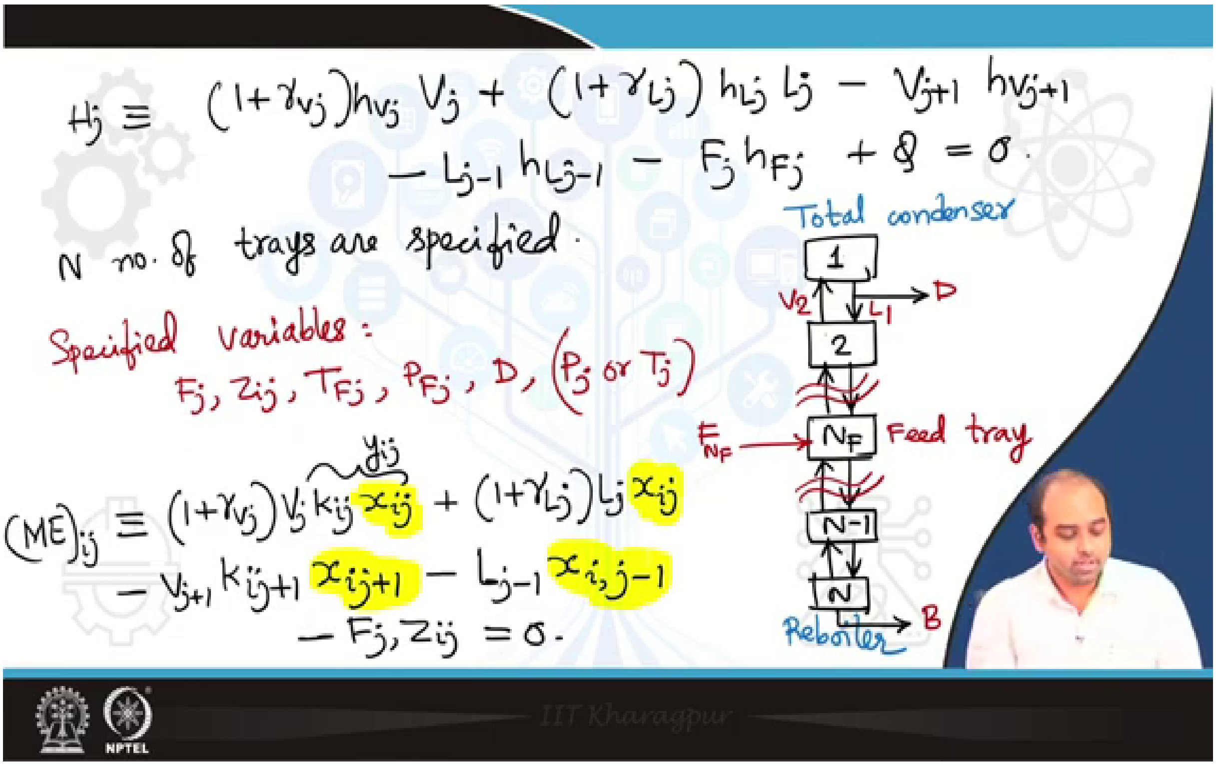

So, for the reboiler, let us also write down for the case of the reboiler, which is the nth stage, so please note the total condenser and the reboiler are part of the stage numbering, this is the reboiler, so for the reboiler we have I hope now this is clear to everyone for the reboiler and you have only the liquid part LN minus 1 x i N minus 1 equal to 0.

So, now in all the equations, if you look carefully particularly the M E equation, if you look carefully the M E equation you will see that you are having so here, you are having terms of x i j, you are having terms of x i j plus 1 and x i j minus 1 and of course z i j, so x i j is the unknown quantity. So, you are having here x i j, x i j plus 1 and x i j minus 1.

So, this M E equation that we have written down can be generalized in this form, sorry generalizing the M E equation as let us say A j x i j minus 1, the coefficient for the j minus 1 component j minus 1 term is a j. Then let us say B sorry I also want to write as a i j and B i j, sorry x i j plus C i j is the coefficient of the j plus 1 term and I can write this as D i j.

So, if I compare the coefficient and this I mean where I can write A i j as L j minus 1, then B i j, the coefficient of the term including x i j is minus of you have 1 plus gamma sorry gamma L j k i j, then you have V j plus L j, so this is not gamma L j gamma V j, L j plus u j. So, if I go back so this is the term so you are having for 1 plus gamma V j, V j k i j that is 1 and then again you are having 1 plus gamma L j, L j, this is the coefficient of j i j x i j parameter.

So, this part I can also write down as 1 plus gamma L j L j, this I can write down and minus is given in front of this equation, because, we are trying to write down both in other way round that is why I have given this as a minus. If you have noted down the j minus 1 term is written down as plus L j minus 1 that is why the B component is minus and C i j is equal to k i j plus 1 into V j plus 1 and D i j is equal to minus z i j F j. So, this is how I can form the A B and the C coefficients for this M i j equation.

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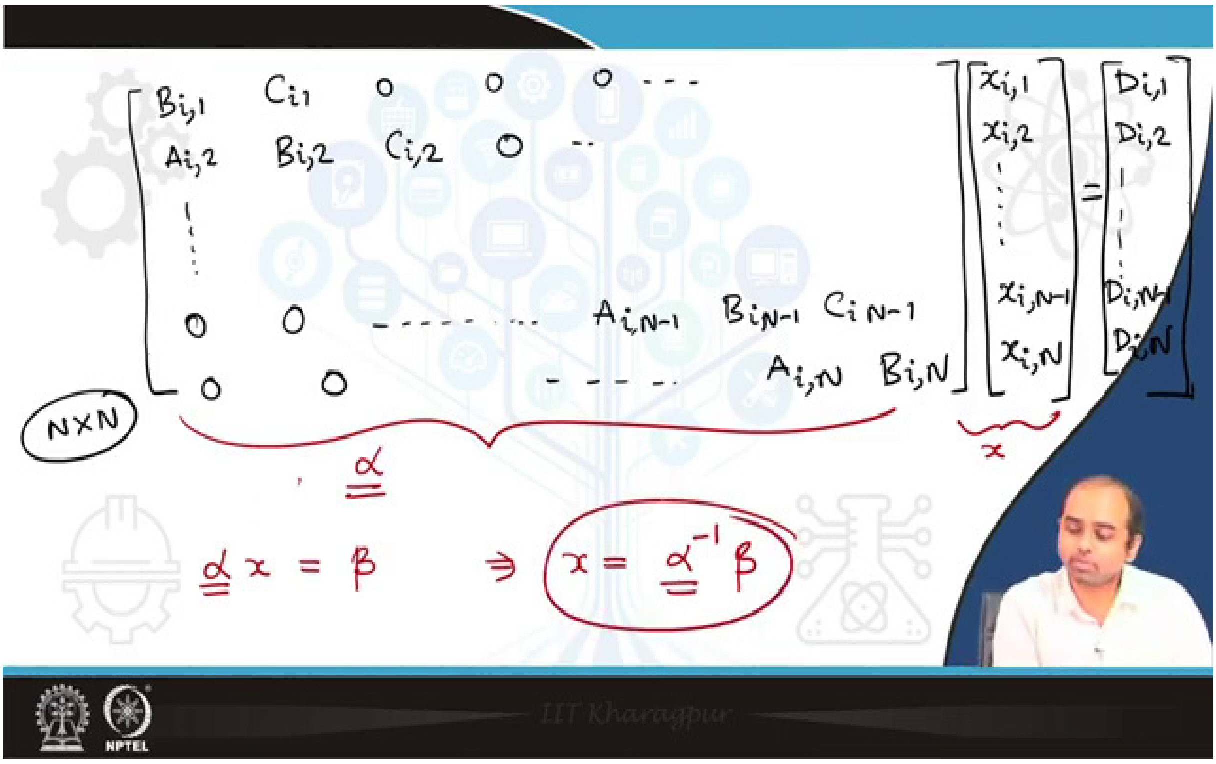

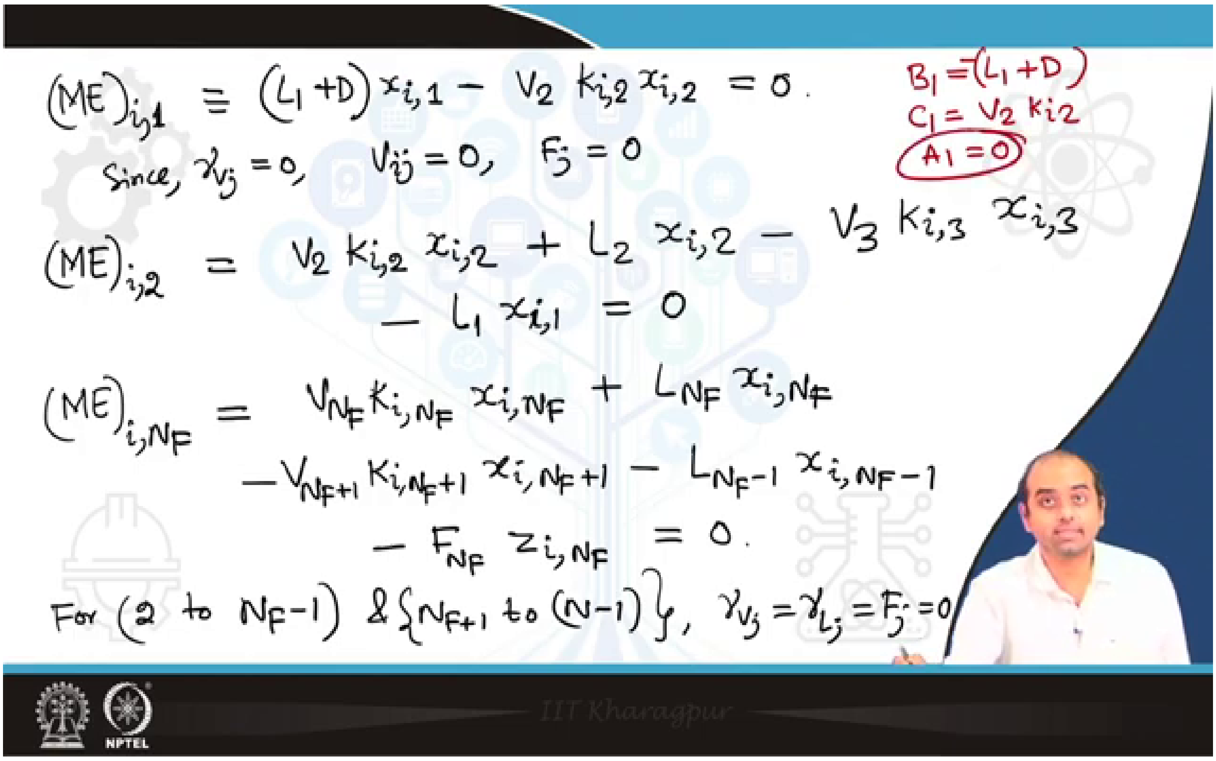

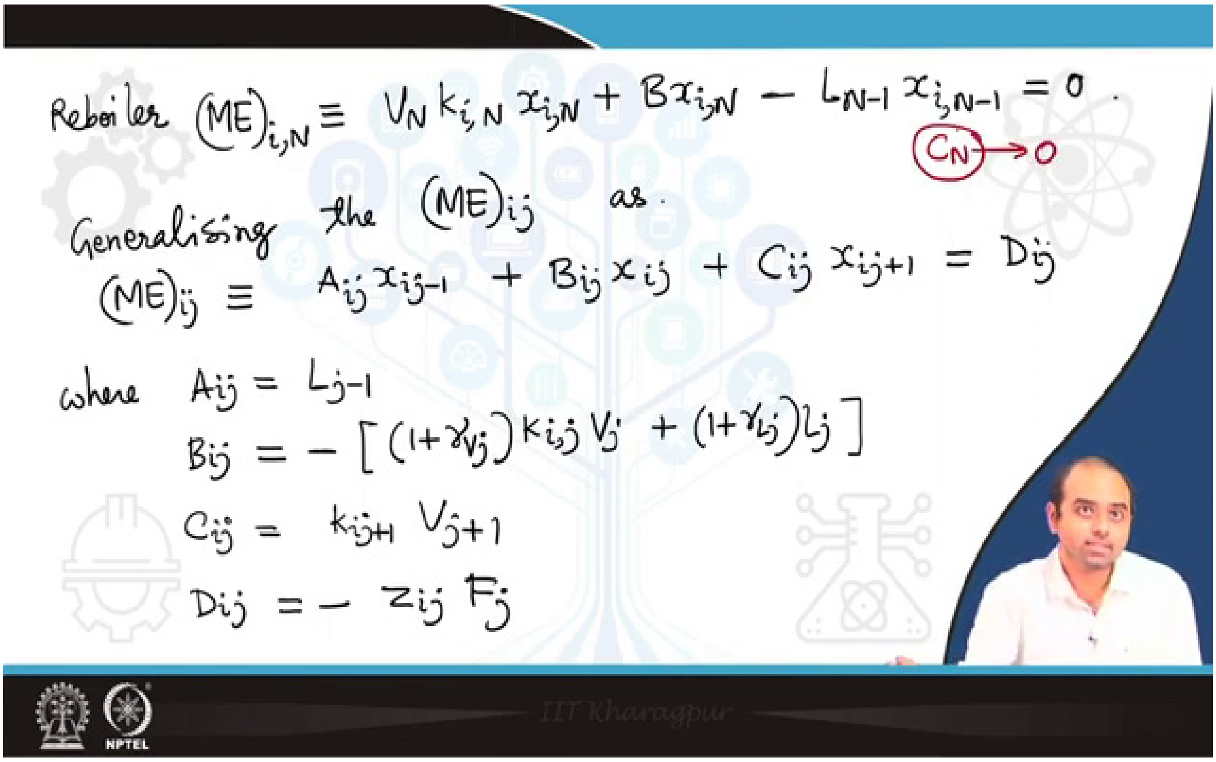

So, if I am going to write down the M E equation for all the individual trays or for all the individual stages what do I get? I get a matrix formulation please note that I will be getting a tri-diagonal matrix, where the tri-diagonal matrix I have the first term as B i 1, C i 1, this will go on. Then I am having A i 2, B i 2, C i 2 and then you have zeros.

So, this will continue and let us write down the N minus 1 stage, so I will be having something like A i N minus 1, B i N minus 1 and C i N minus 1 and the last stage would be a A N sorry, A i N and B i N, so this is the tri-diagonal matrix that we are getting here and of course each of these rows would be multiplied with x i comma 1, x i comma 2, then x i comma N minus 1 and x i comma 1. So, such tri-diagonal matrix forms need to be prepared for all the individual components, this is for 1 component, similarly we will have for other components. And if you recall from the previous case for i so this is N cross N matrix.

So, if you recall here for the stage for the tray 1, you will find that there are no x 0 components, so from here I can write down if I try to write down the individual coefficients I will see that my B 1 is equal to L 1 plus d and C 1 is equal to, so this is minus of this and C 1 is equal to V 2 into k i 2, but A 1 is equal to 0, A 1 does not exist.

And similarly, for the last tray for the reboiler tray, you will see that there is no term that there is no term related to x N plus 1 i N plus 1. So, it means C N in this case is also 0, it does not exist C N does not even exist, it is not that it is 0, but it does not exist here also A1 does not exist. So, this satisfies the structure of the A i N and this tri-diagonal matrix, where for the first row you do not have A 1, similarly for that last row you do not have your C N.

So, in short this can be so this matrix I can call that as alpha and this is the x matrix and that is the whatever beta or D matrix I can write alpha x is equal to some beta matrix, this vector x is a vector and this last column, which we have is a vector. So, x is a vector and B is a vector, so something like this can be written down and I can from here I can find out my x is equal to inverse of this matrix into B, so this is the classical way, but here this is a tri-diagonal matrix system, so the best way is to use the Thomas algorithm.

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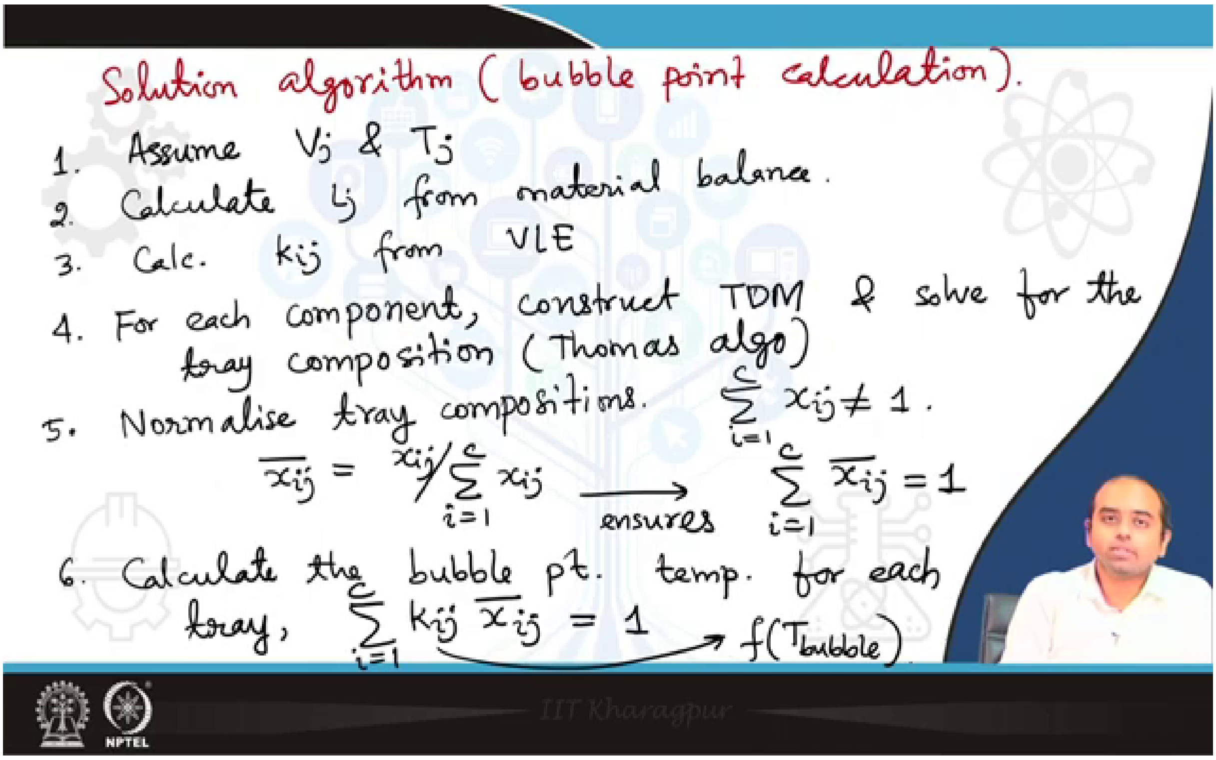

So, now let us talk about the solution strategy what is the solution algorithm here algorithm for this bubble point calculation? So, first you assume the tear variables, so V j and T j are the tear variables for this problem. So, of course you need not to assume both of them, but it is often a useful or it is often helpful if you assume both of them, but at least one of them needs to be assumed, because that out of this V j, L j, T j and P j you have to guess one of these values. So, we are considering that apart from one of these values you guess for two values to begin with.

Next step is – calculate L j from material balance you can easily calculate that for each stage from the material balance. Then calculate k i j from vapour liquid equilibrium, the next fourth step is for each component construct this tri-diagonal matrix and solve for the tray composition, see once you know your L j, V j, P j or something these quantities I mean pressure etc pressure is generally also specified P j is known, then you can calculate out your k i j. And then for in the say expression once your k i j and then V j and T j are already guess parameters or assumed parameters you calculate your L j. So, all the coefficients of the TDM will be known.

So, for each component if there are like let us say 10 components for each case you have to construct a TDM and solve for the individual components in the trace. So, all the component composition in each of the trays will be known by solving this, of course how will you going to solve using Thomas algorithm, otherwise the calculation would be extremely inefficient or slow.

Next is that, this is a very important step, normalise tray composition, please note that whatever the tray compositions that you have got for each of the individual trace, the summation of all the components, I mean by mass balance has to be equal to 1, but since you have already assumed your V j and T j, which are not the actual solution, it is not sure that the summation I mean you cannot ensure that the summation of x i j of over i, not over j, for all the components in each tray, these may or may not be equal to 1. So, better is to normalize them that is the technique.

So, what is the normalization you do that x i bar is equal to x i divided by x i summation over all the components, if you do then it ensures that the summation of this normalized tray composition will be equal to 1, this is kind of normalization. Next is to calculate the bubble point, calculate the bubble point temperature for each tray and how do you do it you use the other summation equation k i j and to get this you use the normalized tray composition, this is nothing but summation of y i j.

But calculation of the I mean this y is you relate it as with the normalized composition, this is equal to 1. So, from here you already know the I mean this in this x i this normalized tray composition, so k i j is a function of temperature, this is a function of the bubble point temperature. So, from there you can work out what is your bubble point temperature.

So, now since this T j and x i j, this whatever are known the tray composition and the tray temperature are known calculate V j, the vapour flow rate in each of the tray vapour flow rate, vapour flow in each tray from the H equation enthalpy equation, because in the enthalpy equation the equilibrium constant is already known from the step 6 you have already calculated out equilibrium relation provided temperature is known equilibrium constants are known, then your V j I mean your V j is the only unknown in that equation.

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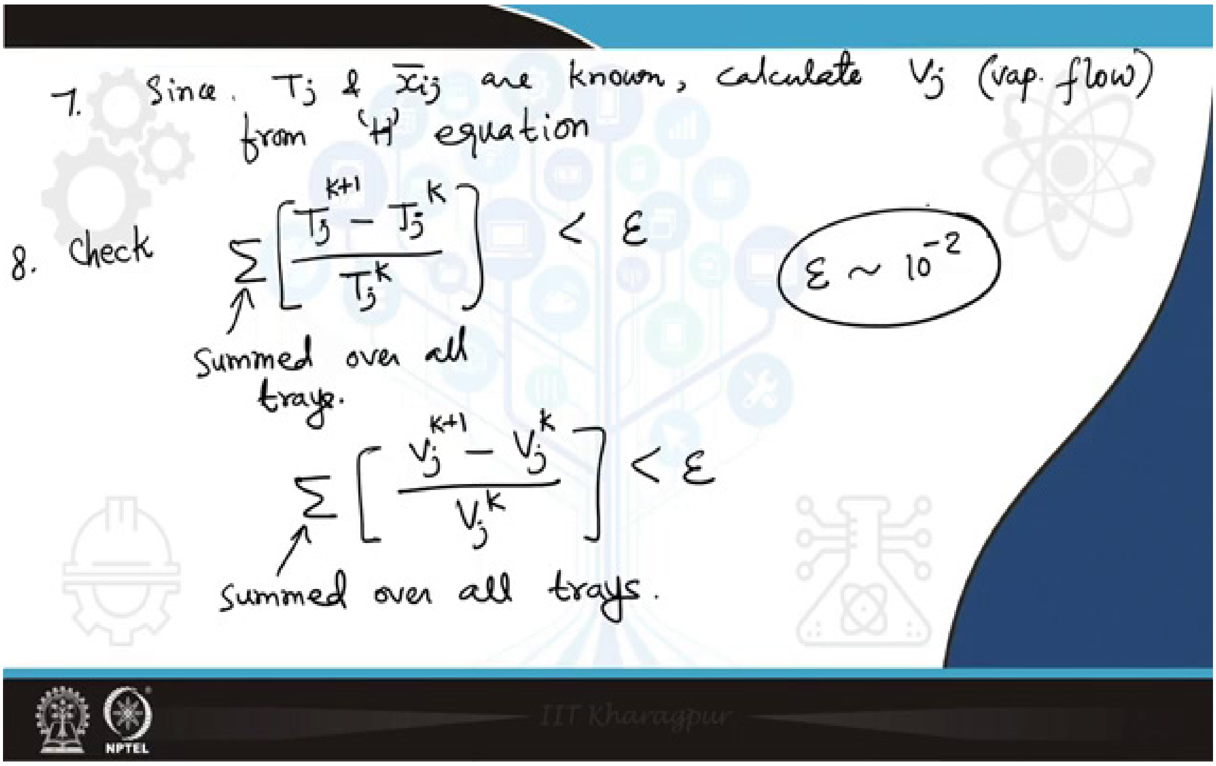

And finally, what you need to do? You need to check that this whatever you have assumed, and whatever you are getting from step 7 are same or different, I mean relatively speaking and this difference or whatever this relative error we call has to be done over all the stage summed over all trays. So, this has to be less than a tolerance.

Similarly, the V j values in this case and whatever you have assumed are relatively they are close or not that is something has to be checked, again summed over all trays. So, what all trays, this if you check this relative error as the difference of the temperature and the difference of the vapour flow rate across all the trays, they has to be less than the specified tolerance.

So, this is the check, if not then this new guess new values of your T j and V j, whatever you got from step number 7 has to be used in the first stage as your initial guess and then you redo this calculation and continue this checking. So, please note that in each of these iterations you have to set up or you have to solve the tri-diagonal matrix and get the individual tray composition and then check for these two criteria, check for the temperature as well as for the vapour flow rate, these two criteria's needs to be checked for convergence and each of them have to be satisfied individually.

So, this is the summation you need to do over all the trays, because all the tray compositions or all the tray values will not be will not may not come same so you have to do the summation, so the relative error has to be summed up and then only it should be below a certain tolerance value. So, typically this epsilon is generally at least it should be less than 10 to the power minus 2 at least, at least 10 to the power minus 2, 10 to the power minus 3 for convergence.

So, I hope all of you had a proper understanding of the solution algorithm of the bubble point method or the bubble point calculations using the rigorous method of the tear variables and this will of course as you understand will give you the understanding or the calculation of the tear variables and the individual tray temperatures their compositions. So, in the next class we are going to work a small example problem, so that it will be more clear on how to put the numbers and how to do the calculations. I hope all of you found this quite useful. Thank you.