Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 33
MESH equations and DOF analysis

Hello everyone in this class today we will work out or we will try to discuss about the mesh equation. So, mesh stands for the material balance equilibrium summation and the enthalpy balance which is very relevant for multi-stage multi-component distillation process and this will form actually once we do the degree of freedom analysis and then possibly from the next class onwards, we will see that this actually forms the basis of the subsequent rigorous methods of the calculations.

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So, let us begin today. So, we will talk about the mesh equations, we will try to make write down these mesh equations in control volume or across a particular stage and then we will also do a degree of freedom analysis for this case across the stages in the overall distillation column. So, let me write out first what does this mesh stands for.

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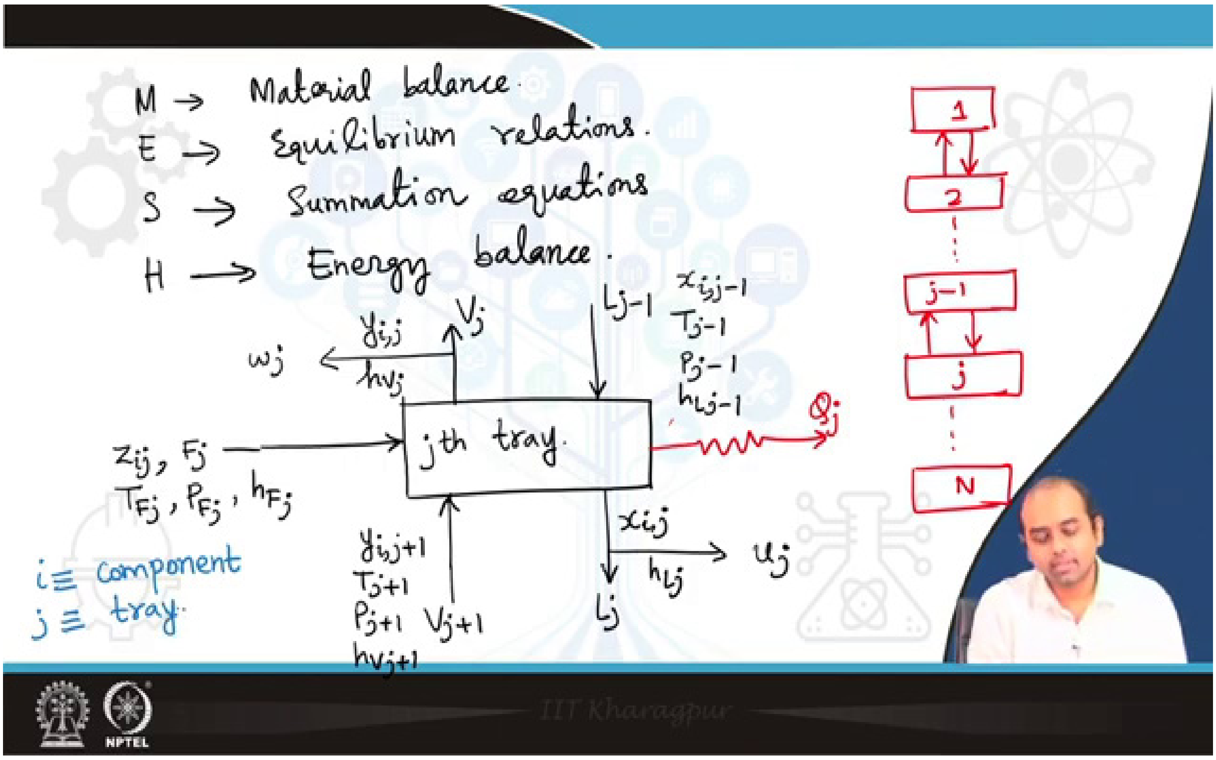

So, mesh represents the material balance, E stands for the equilibrium relations, S stands for the summation equation and H stands for the energy balance. So, with this these equations actually form the basis of all the rigorous calculations, the tearing methods, bubble point calculations, simultaneous correction methods and all.

So, let us try to first write down or have a good schematic of a tray. So, let us call this as jth tray. So, the idea is that any stream which is leaving the tray will have the indices in the form of subscript for that particular j. So, if the stream that is leaving the tray and the vapor part that is leaving that particular tray, we are going to write that as V j. Similarly, the liquid that is leaving this tray will be denoted as L j.

The vapor that, the liquid that is coming into the system is represented as L j minus 1 because the previous tray, the numbering is from the top to bottom, so the liquid which is coming from the top, the previous tray will have a numbering of j minus 1, so the stream that is leaving that tray will have the indices of j minus 1, so liquid is j minus 1.

Similarly, the bottom tray, the tray below this particular jth tray will have index of j plus 1 that is how these are consecutively numbered from 1 to n, from top to bottom. So, the vapor that is coming from the tray below this jth tray will be marked as V j plus 1, so this is the kind of nomenclature we will try to follow.

So, what about the other components? So, there could be, this is like we are trying to make a generalized picture here. So, for each tray we will have this provision of w j as well as will have provision for u j so these w j will be applicable for the top, the bottom and the feed tray and not the feed tray, sorry the top and the bottom and for other cases unless you have some side cuts in the distillation column, these would be will be close to 0, but for the general purpose we define them.

So, let us write down also their composition. So, this is y i, comma j and we also have h V j so this is for the vapor stream that is why I have written down h V j and y i j is the vapor phase composition, for this tray the compositions are x, so this is the ith component at j minus 1 stage. So, please always note the index very carefully and we have h L j minus 1.

Similarly, let us also write down the index for the vapor stream that is entering the system y i j plus 1, then we have T j plus 1, P j plus 1 and we have h V j plus 1. In this case you have x i j and h L j. We can also have a feed stage into this, a feed line or feed stream into this jth tray. So, generally for, only for the trays which have some feed you can have single feed or multiple feeds, this stream will exist and for rest of the trays this will be non-zero, so this you have F j and Z i j is the composition, T F j, then you have P F j and h F j represents the enthalpies.

So, I hope all of you understood the tray layout. So, even let me just write this explicitly, so this is first, then this is second. So, like this it goes on, you have j minus 1, you have jth tray. Similarly, it goes all the way up to N stage, this is 1, 2, j minus 1. So, essentially you can realize that streams which are leaving the particular stage will have their number and that is how we have denoted them.

There is also one important part that it can have some external heating or internal heating whatever so I can write that as Q j, so Q j could be positive, Q j could be negative. So, this completes the nomenclature of the tray and based on this idea the subsequent equations would be developed.

So, please always keep this in mind about the nomenclature of the tray, how do we write the individual variables, the symbols, the designation what the subscript and the superscript, please note that there is no nothing such as V i j or L i j, because V is the total vapor flow rate, L is the total flow liquid flow rate, F is the total feed flow rate that is not for the particular component flow rates.

But x i j, y i j are the component mole fractions that is why i is written down so i and j, i represents maybe I should also write it down explicitly that i represent, so i represent, i represent the component and j represents the tray index. So, now let us move to the material balance equation.

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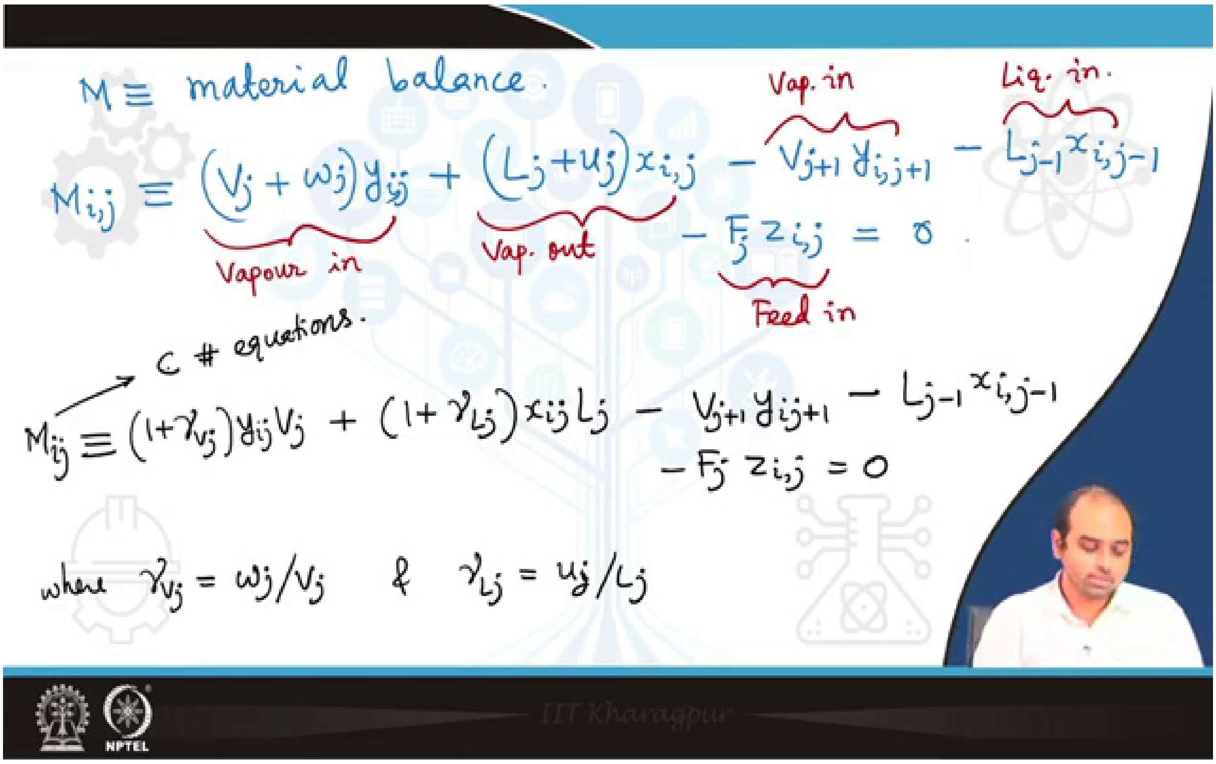

So, M stands for the material balance equation, so the material balance as you know is simple in and out, mass in and mass out both for the vapor and the liquid fractions. So, this is the part that is leaving the stage in the form of vapour, this is the part that is leaving the tray at in the form of liquid and this is equated as V this vapor that is coming into the system, liquid that is coming into the system and feed that is coming into the system, this is the balance equation.

So, let us mark this balance equation as M i, j so just to be specific, so this is the vapor in to the system, this is the vapor out, so this is the liquid, sorry this is the vapor into that particular tray, this is the vapour, sorry liquid in the tray and this is the feed introduced into the system. So, this is the overall material, sorry the component material balance that we have at this particular stage at steady state, understand? So, because at steady state there is no accumulation of any of these components, so this is the balance equation at the steady state.

So, I can just write in little bit modified form as 1 plus gamma V j y i j V j. So, what is this gamma? So, where gamma V is nothing but the ratio actually, gamma V j is W j by V j, so this is the fraction of the flow rate of the total vapor flow rate that is that you are getting in the side cuts. And y i j V j gives you the idea of the component flow rates, component vapor flow rates.

Similarly, L j is u j just a different way of writing. So, x i j L j is the total component liquid flow rate, then you have minus V j plus 1 y i j plus 1 minus L j minus 1 x i j minus 1 minus F j Z i j is equal to 0 and this is what we are calling as M i j equation. So, total there are C number of equations, C number of material balance equations, for C number of components, there will be C number of equations. Now, let us look into the equilibrium relations.

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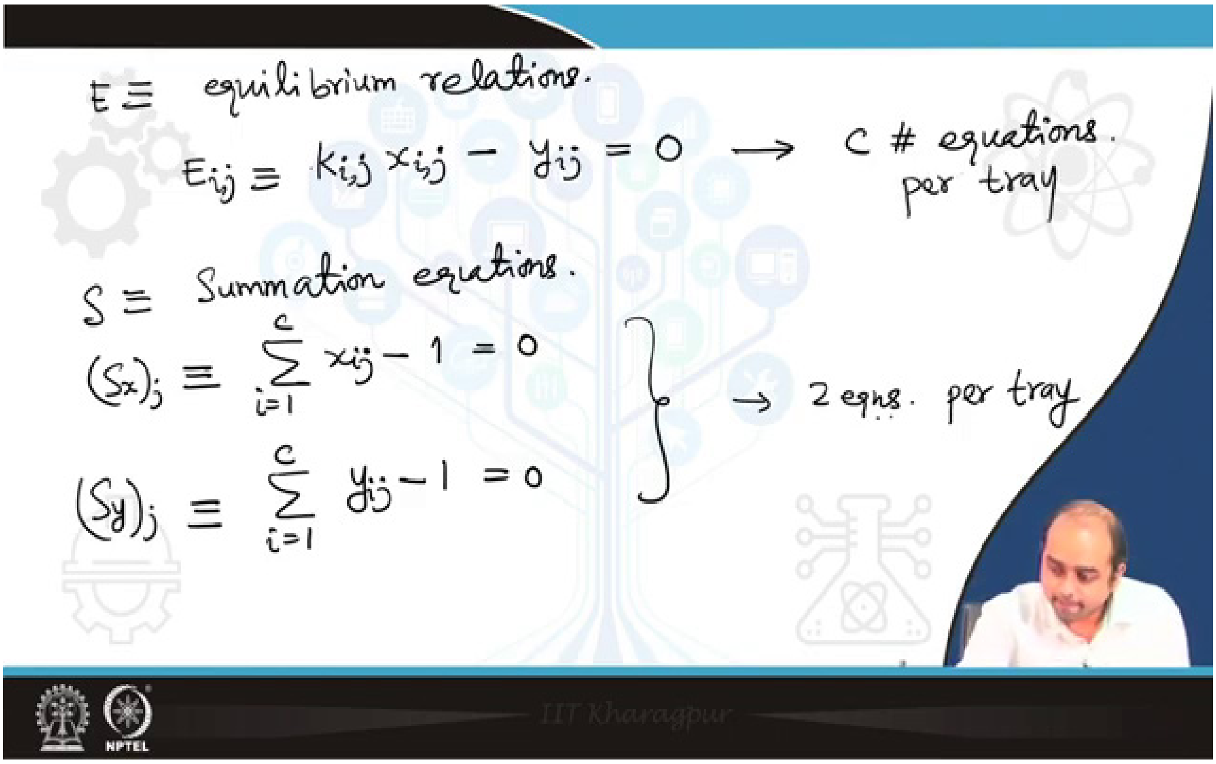

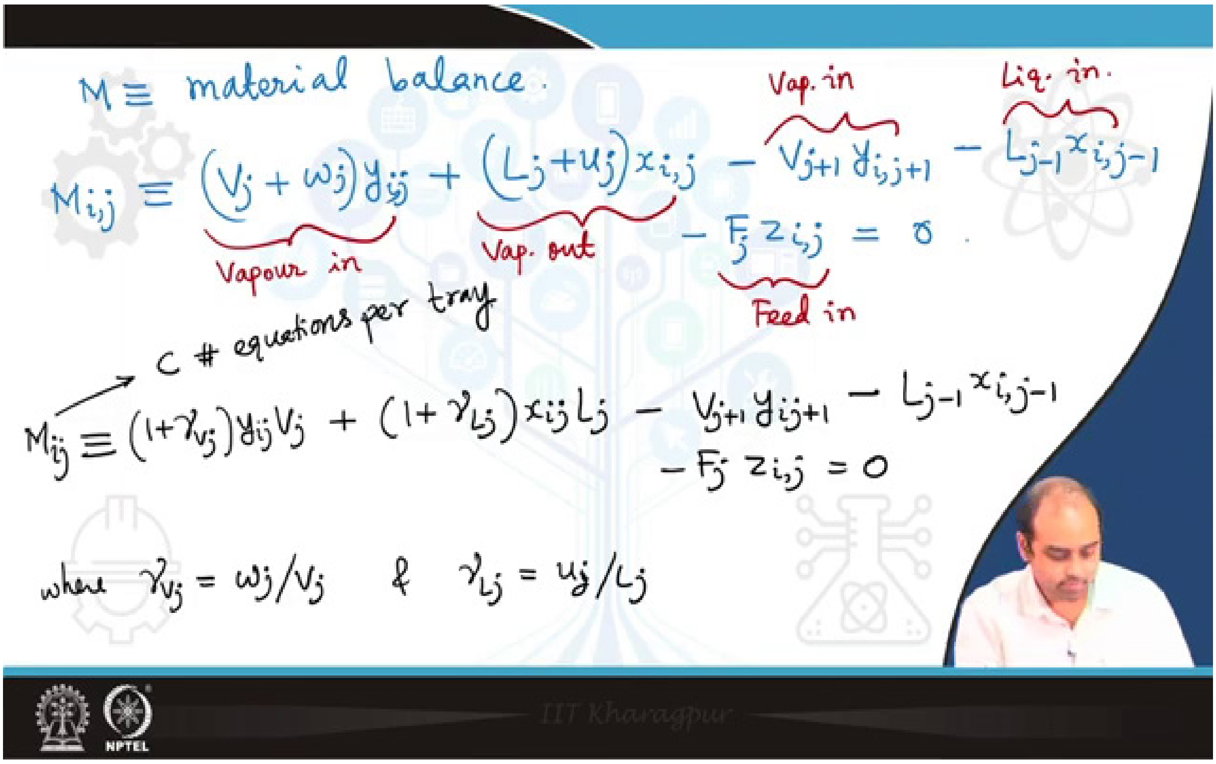

So, E stands for the equilibrium relation, so I can write k i, j x i, j minus y i j is equal to 0 this is what equilibrium relation and this is valid at all the trays. So, from here also you are going to get C number of equations because this will be valid for all the components, vapor liquid equilibrium has to exist for all the components.

Next is the summation equation, for all the components this balance has to hold at each tray, so this two summation equations has to hold and please note since we have not used the overall material balance we can write down two separate summation equations like in the previous case when we discuss, when we were discussing about the flash distillation we said that since we have written down the overall material balance these two summation equations are clubbed together and one only one summation equations were available to us.

But here we did not use the overall material balance, in the material balance its all individual component balances that is why we got C equations there. So, now in the summation equations we can use these two separate summation equations. So, from here essentially you are getting two equations, two equations you can get per tray, of course. So, here also C equations part tray, here also C equations part tray.

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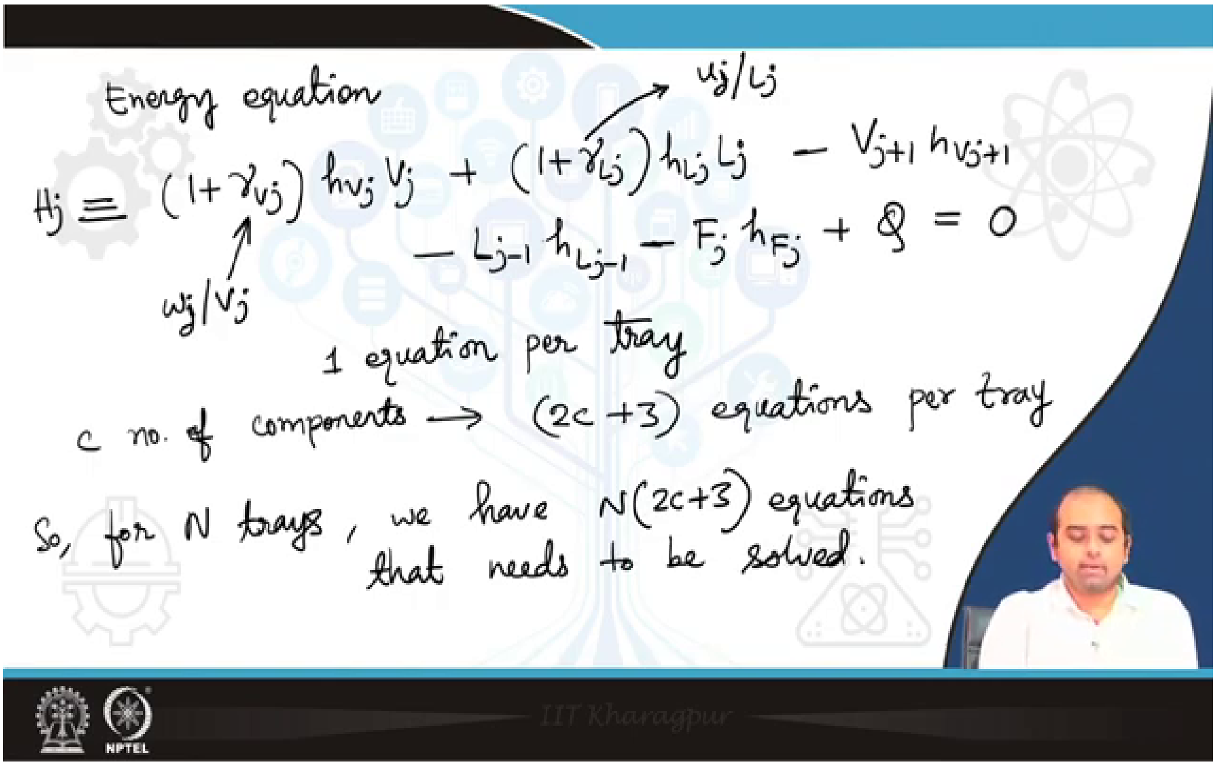

Now, we are moving ahead, now let us talk about the energy equation. So, energy equation we use that same gamma form write h V j so this is the energy into the system in the form of the vapor and this is in the form of the liquid and then we have energy going out or the enthalpy going out, this is the liquid part, enthalpy of the feed and the external heat supplies.

So, this is your H j part and please note that of course gamma I hope all of you remember it is W j by V j and gamma for the liquid is u, so this is the ratio of the side cuts. So, this is the enthalpy that is we are balancing the enthalpies here in minus out again but please note that this enthalpy balance is only, there is only one equation per tree for, from the enthalpy balance.

The enthalpy balance does not hold for each of the component, it is only one total enthalpy balance, one equation per tray. So, then for C number of components what we get? C number of components we have 2 C plus 3 number of equations per tray. C number of material balance equations, C number of equilibrium equations, two summation equations and one energy equation, so total you are having 2 C plus 3 number of equation. So, for N trays, we have N into 2 C plus 3 number of equations, that needs to be solved.

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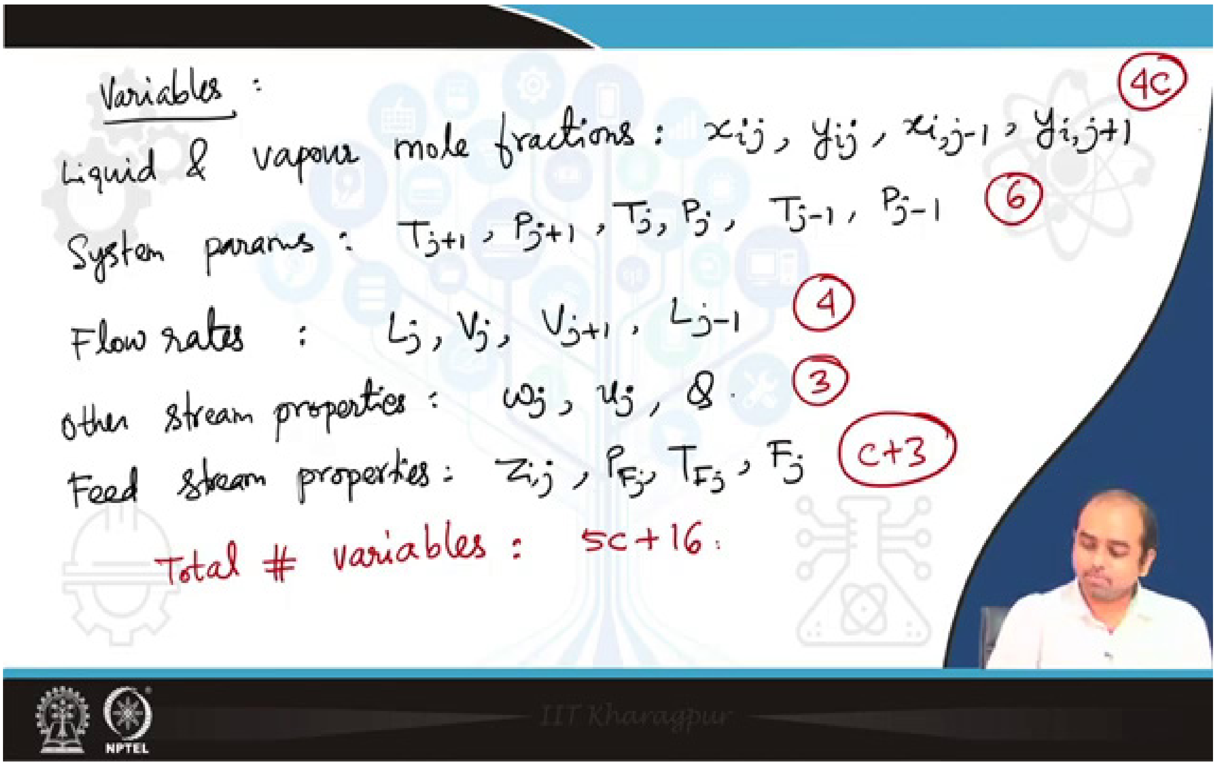

Now, let us look into the number of variables in this system because the number of variables has to match with the number of equations, at least or whatever the degrees of freedom that we have should also be specified and once we list down the number of variables it will be easier to estimate the degrees of freedom.

So, for each tray the liquid and vapor mole fractions are the variables, so let us list them down. So, you are having x i j, then y i j, x i j minus 1, y i j plus 1, then we have the system parameters, so that is t j plus 1 then you have p j plus 1, so this is for the bottom tray liquid for the liquid part these are the bottom conditions that are coming in for the bottom stream.

Then you have T j P j and you also have T j minus 1 and P j minus 1 so these are the streams for the, from the stream, from the top streams or the stream that is entering to the system vapour streams these are their conditions. Flow rates you have L j, V j, then you have V j plus 1 this is the vapor flow rate from the bottom tray, top tray and the, sorry bottom tray and L j minus 1 is the from the bottom tray we are getting.

So, next is other stream properties it is w j, u j and Q. Feed stream properties are composition, pressure, sorry this is I should not write Z i j, sorry yeah Z i j then i have P F j, T F j and I have F j flow rate so let us count the variables now. So, from here total number of vapor and the mole fractions you get these are like for each of the components so it is 4 C number of, 4 C number of variables you are getting from here.

Then from here you are getting 1, 2, 3, 4, 4 variables, here also 4 variables, sorry system parameter is 6 variables I have written down it 4, flow rates are 4, other stream properties are 3 and feed stream is C plus 3 because C compositions are there for individual components, so total number of variables, total number of variables in each tray is 5 C plus 16.

So, please note we do not consider the H or the enthalpies because they are related to temperature and pressure and since already, we have considered the temperature and pressure for this problem and for this system we do not again write down the enthalpies because they are function of temperature and pressure, so they are not explicit variables, that is why they are excluded, the total number of variables is 5 C plus 16.

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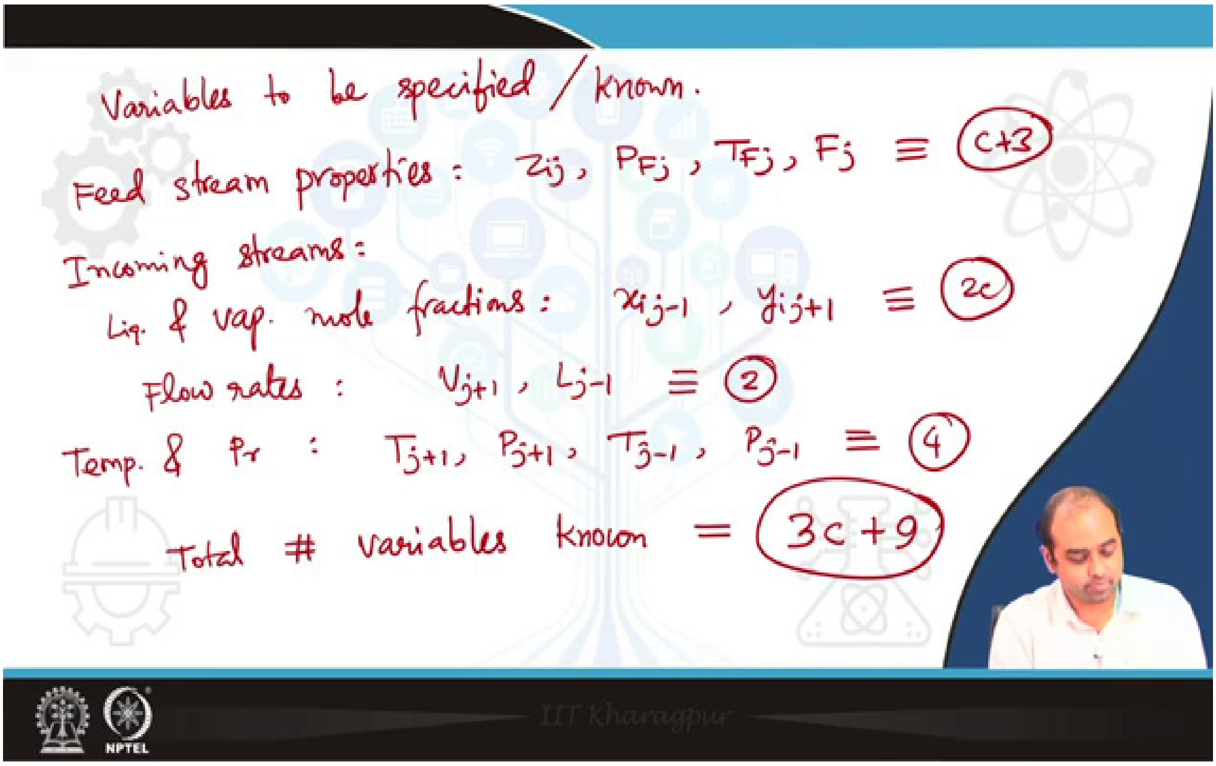

Now, let us see what are the variables are to be specified or known, variables to be specified or known in this system. So, liquid, first is the feed stream properties, these are generally known feed stream properties, for any tray these should be known. So, what are these? Z i j, sorry P F j, T F j and you have F j, so here C plus 3 number of variables which is known. Then you have incoming streams, this is very important, so all the incoming stream properties would be known because they are part of the solution of the previous tray, either the bottom tray or the top tray corresponding to the jth stage.

So, any stream which is coming from j minus 1 or j plus 1, their properties would be known because they will be solved as a part of their stage calculation so we cannot double count them. See if the unknown streams for jth tray, the stream properties would be T j, P j, L j, V j, x i j, y i j, so similarly that is the case for the previous stage also. So, in the previous stage also these are unknown which are solved as a part of their calculation of that stage calculation.

So, T j minus 1, P j minus 1, then x i j minus 1, x, then y i j plus 1, all these would be known because they are coming from the previous tray. So, from the incoming streams the liquid and vapor mole fractions are known. So, this x i j minus 1 and y i j plus 1 are unknown because they are part of the calculations of those stages which is something we do not double count them here because they are known quantities, they are not unknown here, they were unknown in their respective stages. So, in the for the j minus 1 stage x i j minus 1 is an unknown variable but it is not unknown variable in jth stage that is a known quantity because that is already solved in the j minus 1 stage.

Similarly, flow rates of the incoming streams that is V j plus 1, then L j minus 1 are known, so here from here you get two variables known, temperature and pressure, temperature and pressure of the incoming streams that is T j plus 1, P j plus 1, similarly, T j minus 1 and P j minus 1, these are also known because they are also solved as a part of their previous stage calculations, so they are already known quantities in the jth stage. So, total number of known variables are which are known are 3 C plus 9, these number of variables are already known in the system.

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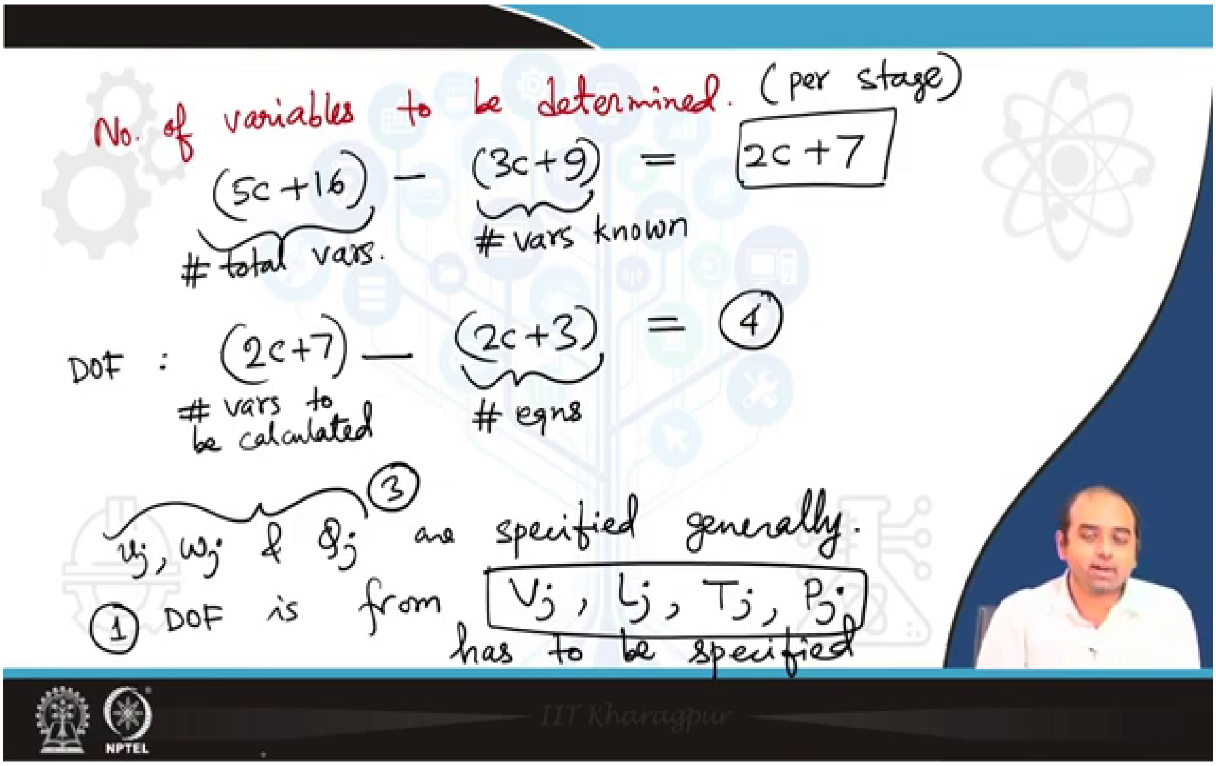

Now, number of variables to be determined, is 5 C plus 16 are the number of variables and already you have 3 C plus 9 number of variables known, so you have 2 C plus 7, so this is the number of variables known and these are the number of total variables in the, in one stage, in the particular stage.

So, this many 2 plus C number of variables are unknown. So, what is the degree of freedom? So, you have 2 C plus 7 number of unknown variables or to be determined variables so these are the number of variables to be known or to be calculated, their values need to be calculated minus 2 C plus 3 number of equations that you have we have already listed down, the number of equations that is 2 C plus 3, so these many number of equations per stage we are trying to say, so everything is per tray or per stage.

So, you are having 4, so there are 4 degrees of freedom per stage in this case. So, usually to accommodate these 4 degrees of freedom this u j and w j which are the side cuts they are known quantities. So, u j, w j and Q j whatever this heat are generally specified, are specified generally.

So, which leaves only one unknown quantity which at least one other parameter or one other variable has to be defined, so these could be, so this, these three are generally specified and most cases u j, w j are 0, Q j something which is external heat supply which is also specified, you know as a part of the operating condition.

So, one more variable or one degree of freedom is from either V j or L j or T j or P j has to be specified, has to be specified, for this to be a unique problem, you cannot work with a system where the number of unknowns are more than the number of equations or the number of equations are more than the number of knowns, in both cases you will get, you will not get a unique solution.

So, one degree of freedom either from these four quantities V j, L j, T j or P j has to be specified and we will see that this forms the basis of the calculation of the tearing methods that how you use them or how you use this idea to solve for the calculations providing that one of them is initially known in the calculations and this is the reason why it becomes iterative calculation.

Because the none of these is known to you so you have to guess them to make it a closed problem and then do an iteration for finding out that guessed value or whatever has been assumed. So, unless this is specified, this one degree of freedom is specified the problem is not closed, the number of equations are less than the number of unknowns that cannot be solved and mathematically it is impossible.

So, we can only solve if one of them is known or specified, so and that, but these are all unknowns in the calculations, in the stage calculations, so one, to know one of them or to specify one of them you have to take a guess and that again, that is where the iterative calculation starts because this guess is not the correct guess, so to correct it you need to do iterations and that is how the iterative calculation evolves.

So, I hope all of you get a fair understanding of the degree of freedom analysis for this problem, for this system of the rigorous method and I hope all of you will, and as we move in the next class and talk about the tearing methods you will realize that how one of these unknown quantities is or one of the degrees of freedom unknown degree of freedom is specified and that is the iteration, iterative calculation actually starts from there. So, see you all in the next class with the tearing methods. Thank you.