Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 36
Simultaneous Correction Method

Hello everyone. In this lecture we are going to talk about another method of calculating the stage calculations, this multi-stage multi-component process known as the Simultaneous Correction Method.

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So, in this simultaneous correction method, we will be encountering something known as the Block Tridiagonal matrix. So, it is a higher version of the tridagonal matrix where individual items or individual elements of this matrix are itself another tri diagonal matrix and you will see that how this is forming.

So, the equation is formulated all together. So, once we write it down, it will be more apparent or more clear. But at least please realize that it is now a block tri diagonal matrix we are talking about. So, how do you begin, I mean to work out the formulation.

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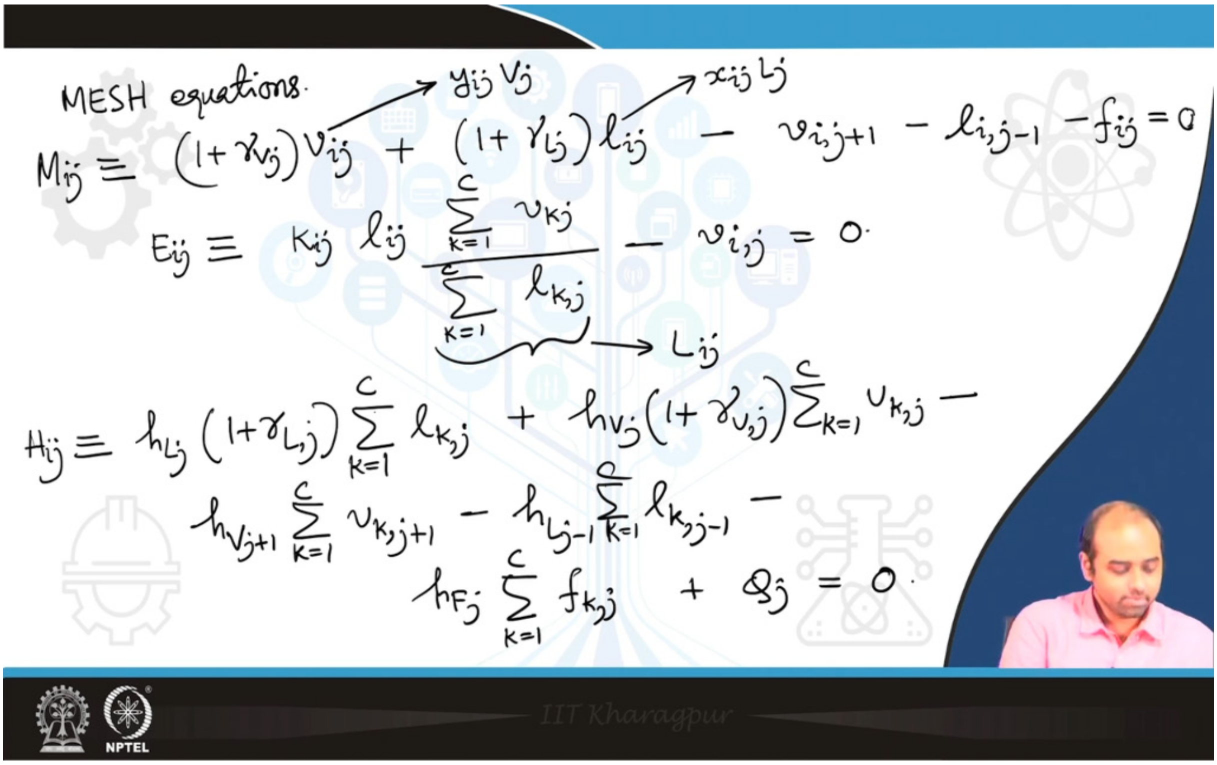

We once again start with our mesh equations. So, you have the M i j as the material balance equation. Please, note that I have substituted this y i j v j as the component flow rate. So, instead of writing the total volume vapor flow rate and the mole fraction in each of the trace, I write the component molar flow rates is a slight modification I made.

Similarly, this is also the component molar flow rate I mean the liquid flow rate which is nothing but x i j L j, okay. Then I also write here as in terms of molar vapor flow rate same way for the liquid and same way for the feed. Similarly, E i j this equilibrium equations are also written down in terms of the individual component flow rates.

So, instead of writing the capital V, I can also write as the individual component flow rates something like K, where I can write K is equal to 1 to C, all the individual components, is not it? I mean, this summation v i j is nothing but capital V j. Similarly, this L k j is nothing but summation of all the component flow rates minus v i j is equal to zero.

So, this is nothing but capital L i j, summation of all the things. Similarly, the enthalpy equation is written down as instead of writing total flow rate, liquid flow did I write the component flow rates. So, in a way I am including all the summation equations into the problem by writing down the component flow rates.

So, you will be having some more terms, hL j minus 1. So, this is the enthalpy balance equation. So, the key thing that we did here is that instead of writing down X and Y or the individual mole fractions, we have written down in terms of the component flow rates, whether it is a vapor or it is the liquid part, we have written down as the component flow rate. This is something we have written it down.

Now, that essentially, we have 2 C plus 1 number of non-linear equations in this case. And 2 C plus 1 number of variables per stage. So, let me write it down also here.

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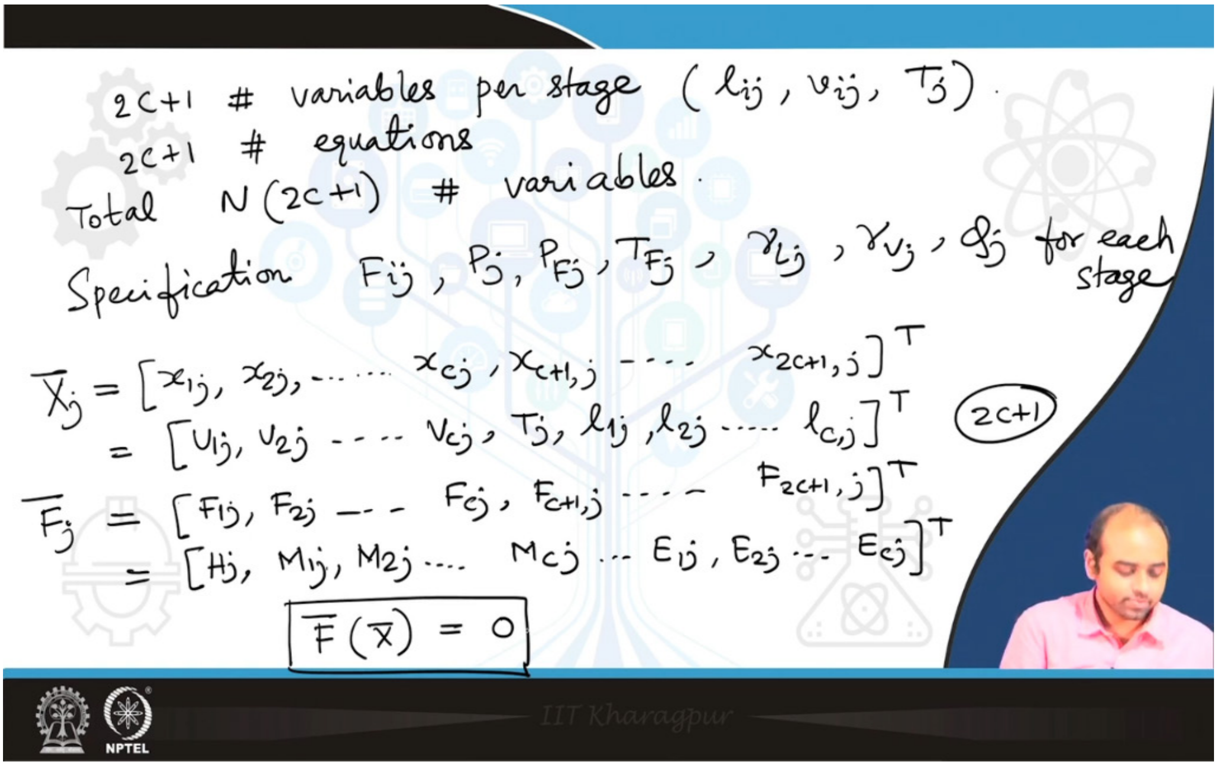

So, you have 2 C plus 1 number of variables per stage. What are the variables? The component liquid flow rates, component vapor flow rates and T j. Number of variables and you have 2 C plus 1 number of equations. One M equation one, I mean, C numbers of M equations, C number of E equation and then one enthalpy equation, total 2 C plus 1 number of equations.

So, it is a matching system now. So, total essentially you are having almost n, not almost, n into 2 C plus 1 number of variables. This is the total number of variables that we are having in this system. Now, what is specified? Generally, the feed components, all the feed properties, this gamma L j gamma v j q j etcetera for each stage is generally specified.

So, let us define this vector X j capital X j as all the number of variables. So, let us say the components are x 1 j x 2 j plus dot dot, not plus, sorry, is a vector dot dot, we have x C j then x C plus 1 j, sorry, almost up to x 2 C plus 1 number of variables, like this. So, which is essentially nothing but our all the v. So, you have C number of V or the vapor component, vapor flow rates.

Then let us talk about the T j and then we have the L 1 j, L 2 j and the remaining entities L C j, it is a total, what how many you are having 2 C plus 1 number of elements in this x vector. And let us also define something as F j as F 1 j, F 2 j. So, these are the individual equations that we are defining.

So, again you have 2 C plus 1 number of equations. So, which are essentially let us say the first one is h j then we have M 1 j, M 2 j like that you are having M C j then you have E 1 j, E 2 j, E C j. So, 2 C plus 1 number of the function variables. Now, with this system, where you have F j as, I mean, F as a function of, I mean, is capital F as a function of capital X. You are ultimately having F as a function of X. So, F is a non-linear system of equations.

So, ultimately, I am having this thing. This is my equation. So, I have a function. Since it is a system of equations, I chose to write them in a vector form. Now, how do you find the roots of this equation? Root of this non-linear equation. Of course, in the system of equation. But how do you generally find the root of the equation? We use the Newton-Raphson method.

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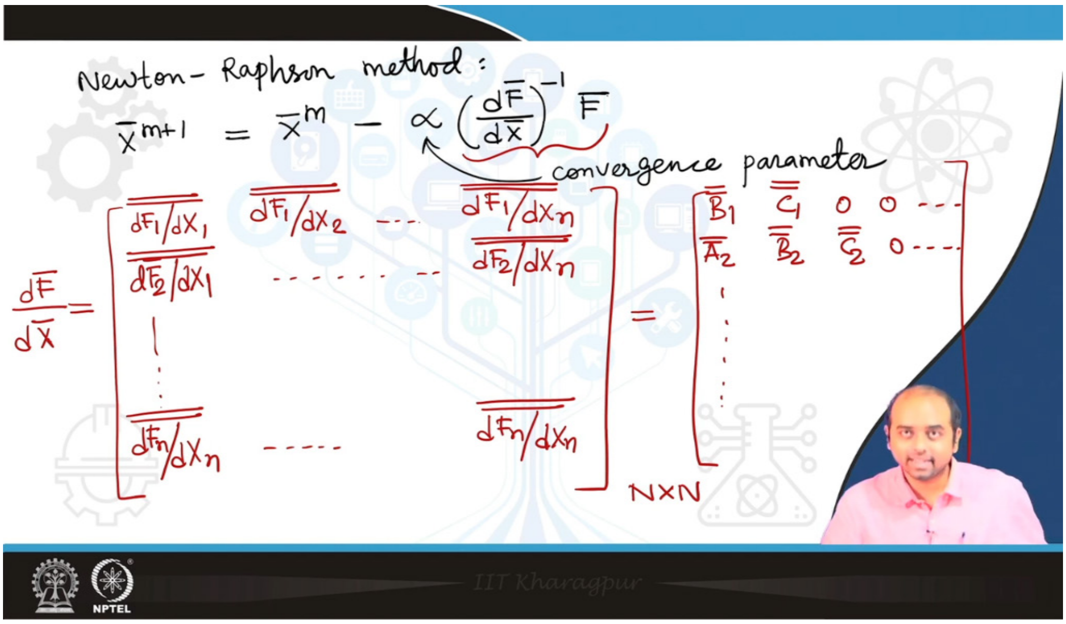

So, we use the Newton-Raphson method, even whether it is a single equation or whether it is a system of equation, we use this Newton-Raphson method. That is a very popular technique of root finding of non-linear equations. And what is this equation? So, this equation, I mean this Newton-Raphson equation tells you that the new, this let me write it this way, is equal to X m minus alpha, this d F d X inverse, these are all bar and just bar, let us write them as bar.

So, this is what the Newton-Raphson equation, for that you need to find out what is your, the derivative and then multiplied with F. So, F divided by the derivative of F that is like the new correction to the previous value of your X. And of course, here alpha is sort of the convergence parameter.

You can choose or a very high value of alpha, a very low value of alpha depending on the nature of the calculations. If alpha is too high then it will force the equations to come quickly towards the solution in low number of steps. But the disadvantage is that it can lead to divergence and you can overshoot your root. So, this alpha is like the controlling parameter to control this correction.

So, this part essentially that you are having here is nothing but the correction to the guess and alpha is the controlling parameter that how much correction do you want in each iteration. You can, if you put in too large number or too have big number; the advantage is that it will need fewer iterations to come closer to the convergence.

But if it is again the downside is that if it is too large, it may overshoot the root or closer to the root or near to the root, it may overshoot that location and it may again lead to divergence. So, here you realize that you have to calculate it out. You have to calculate this d F d X matrix.

So, essentially, you are having this d F d X that needs to be worked out. So, F is a vector, X is a vector, so, if you do d F d X this will lead to a matrix. So, you will be getting something like d F 1 by d X 1. Similarly, the next one would be d F 1 by d X 2, like this it will go on the, first row would be d F 1 by d X n.

Similarly, next column would be d F 2 d X 1. So, like this it will go on. It will be d F 2 by d X n. So, all these are bars because these are vectors. With each vector you have to do this, sorry, F 1 is not a vector but essentially this is a quantities that you need to work out. Let us put them as bar.

So, like this it will go on. So, the last row would be d F n by d X n. Similarly, this would be d F n by d X n. So, this is the matrix you are going to get something like the Jacobian matrix. So, this is n cross n matrix. And please note that F 1 whatever this F 1 we are having, this includes all the components 2 C plus 1 number of components.

So, this one whatever this one I am getting or this X 1, I am getting is actually for stage 1 but again stage 1 involves 2 C plus 1 number of components. So, that is how each of these elements becomes another matrix. That is why I put in double bars. These are not vector or individual components.

This is also small matrix because F 1 is the equation F 1 is the vector for stage 1 and that contains 2 C plus 1 number of elements. So, everything has to be again differentiated with respect to the X variable. So, let me not write down small X, maybe this is it is better to write that as capital X to avoid any ambiguity. Then again F and X contains 2 C plus 1 number of elements.

And if you work this out closely, you will see that this will also follow the tridiagonal pattern. So, here also I can write the first component B 1 which is again a matrix. This is C 1. Like this I can also write A 2 B 2 C 2 like this I can go on writing. Ultimately, I will be getting this A and B and C and at the end I can write it down like that.

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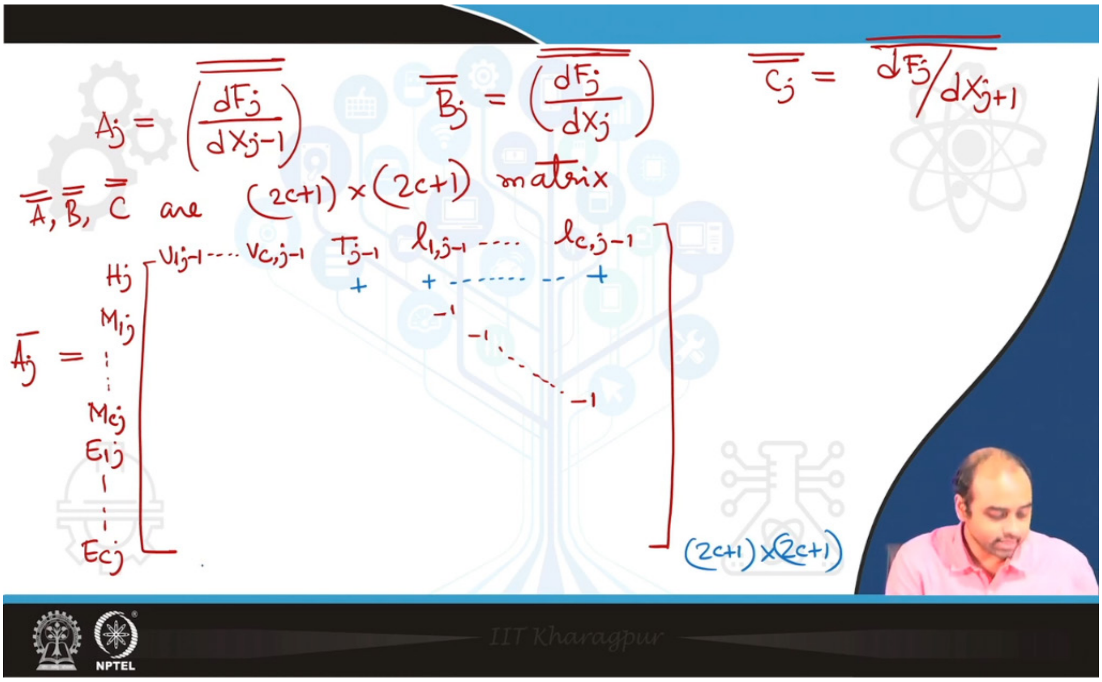

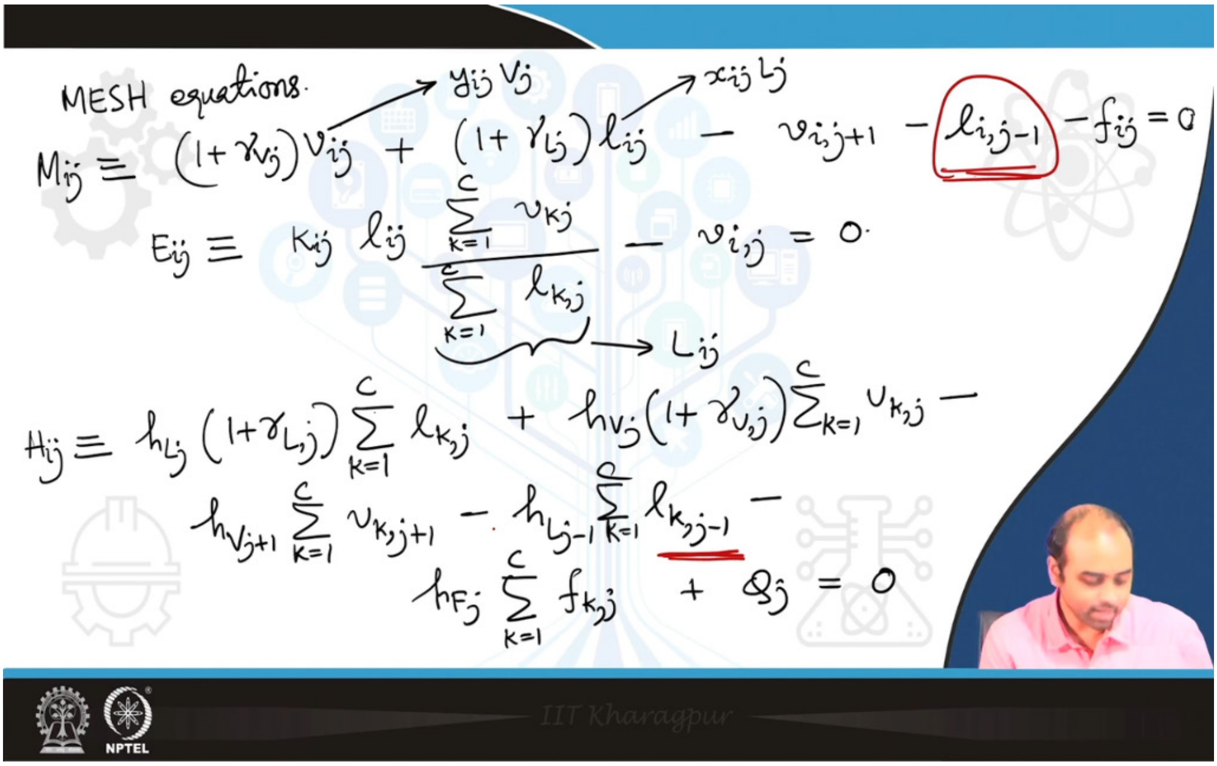

So, where I can write down here A j as d F j d X j minus 1. This is my A. The general description of A, B and C matrix. These are the diagonal elements, okay. So, this is the A, B and the C matrix. And please, note that all of this will constitute that block tri diagonal matrix where individual elements are essentially forming the blocks.

So, the block tridiagonal matrix exists because each of these elements has 2 C plus 1 number of rows and elements 2 C plus 1 cross 2 C plus 1. So, this all these A, B and C. So, A, B and C matrix that we are getting are 2 C plus 1 cross 2 C plus 1 number of these rows and column it is having. And together it forms that big block tridiagonal and the big block tridagonal is fed to the operation of the Newton-Raphson method.

So, in this method, as you see here like in the previous one, we used to do the block tridiagonal for each of the individual components. But here, we are doing it all together. So, you do not need to do it for each of the individual components, they are already incorporated in the individual elements of the block tridiagonal matrix in the form of 2 C plus 1 number of elements in each of these block elements.

So, in calculation in one evaluation of the block tridiagonal matrix you can get one correction to the Newton-Raphson method but whereas in the previous Bubble Point method you need to do the individual tridiagonal matrix for each of the components, work out the tray composition of each of the individual components and then feed it to the iterative step.

But here, you are doing it all together in this one big block matrix. So, what is the typical structure of this A j? So, this typical structure of this A j matrix would look something like this. So, let us say this is like h j then you have M 1 j up to M C j then you have E 1 j and it goes all the way up to E C j. So, that is how total number of these elements you are having.

And here row wise, it would be V 1 then j minus 1. It will go all the way up to V, let me write it down properly, V C j minus 1. Because A j is d F j d X j minus 1. So, all the j minus 1 variable will be coming. This is then T j minus 1 and then you are having L 1 j minus 1 all the way up to L C j minus 1.

So, if you look into the individual equations, if you look into the individual equations, you will see that only this part, only the M versus L equation, if you look carefully into the equations here, the M equations, you will see that for the M equations it contains the L j minus 1 term only. So, a derivation, it is what this this matrix tells you that d M 1 versus, I mean, d M j versus d this L i j minus 1.

So, there are no j minus 1 component in this equation. So, for the M, it is only for the M part of the equations, only the coefficients for the L j minus 1 will exist. So, here if I am going to write in this here, it is only for the M equations that I will see that only they are minus 1 like this. It will go on all the way up to whatever the number of M equations we are having.

And for the h equations, if you see here for the h equations, you will be only having this L j, I mean, L j minus 1 because you are having this L j minus 1 terms here. And there is no V j minus 1 or V j plus1, I mean, this there is no V j minus 1 terms here. So, all the V j minus 1 components should be zero.

It is only L j minus 1 which is there. And you will be having this h i j with respect to the temperature. Because K i j is also part of the system. So, that is the reason, I mean you will also find because of this L A h j minus 1 term present in this equation, the derivative of d h j with respect to T j will also exist but it will not be 1 or something, it will be some value.

So, let us mark those values in this case as like some quantity. So, this would exist and this T j would also exist. So, this is the general, so, rest will be zero. Because there is no derivative possible with V j minus 1 quantities. And also in E j, you do not find any J, V j minus 1, T j minus 1 or L j minus 1 components.

If you look into the E equation, it is all L j V j these things, there is no j minus 1 component. So, with respect to E everything would be zero. So, that is the reason why we will see that rest of the terms of this matrix is equal to zero. So, this is a 2 C plus 1 cross 2 C plus 1 matrix.

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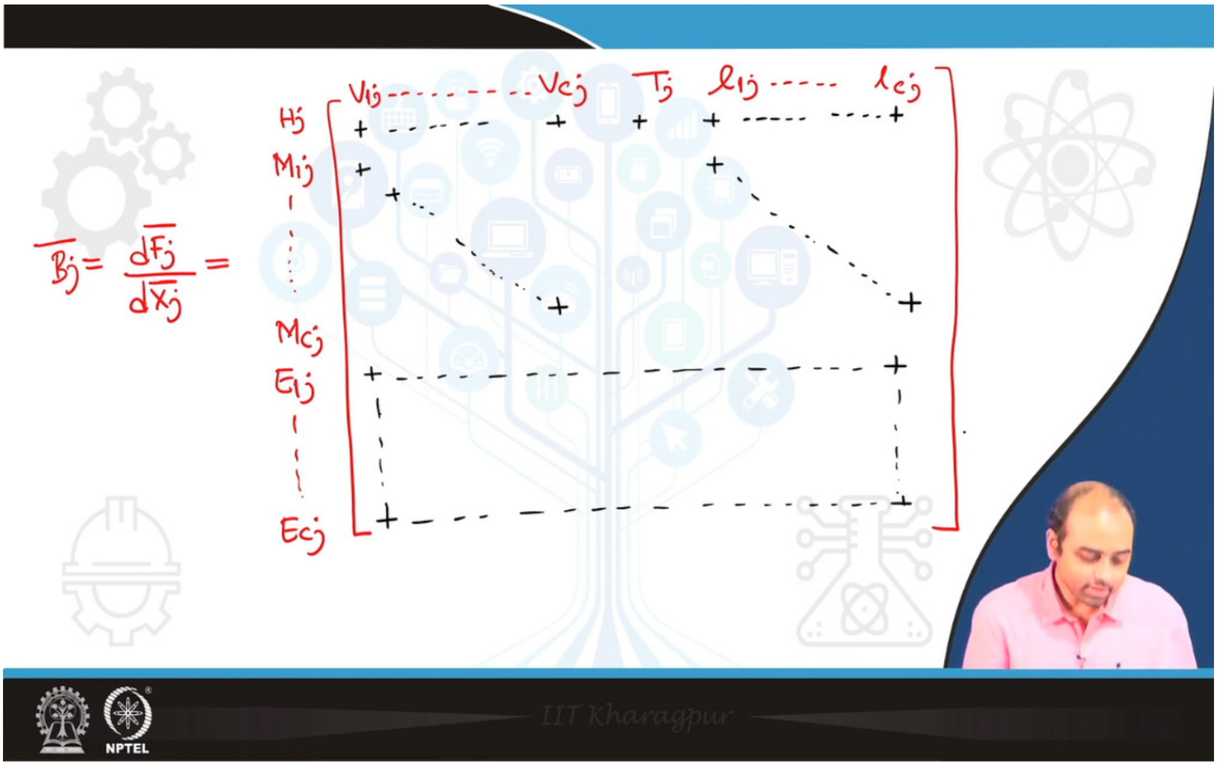

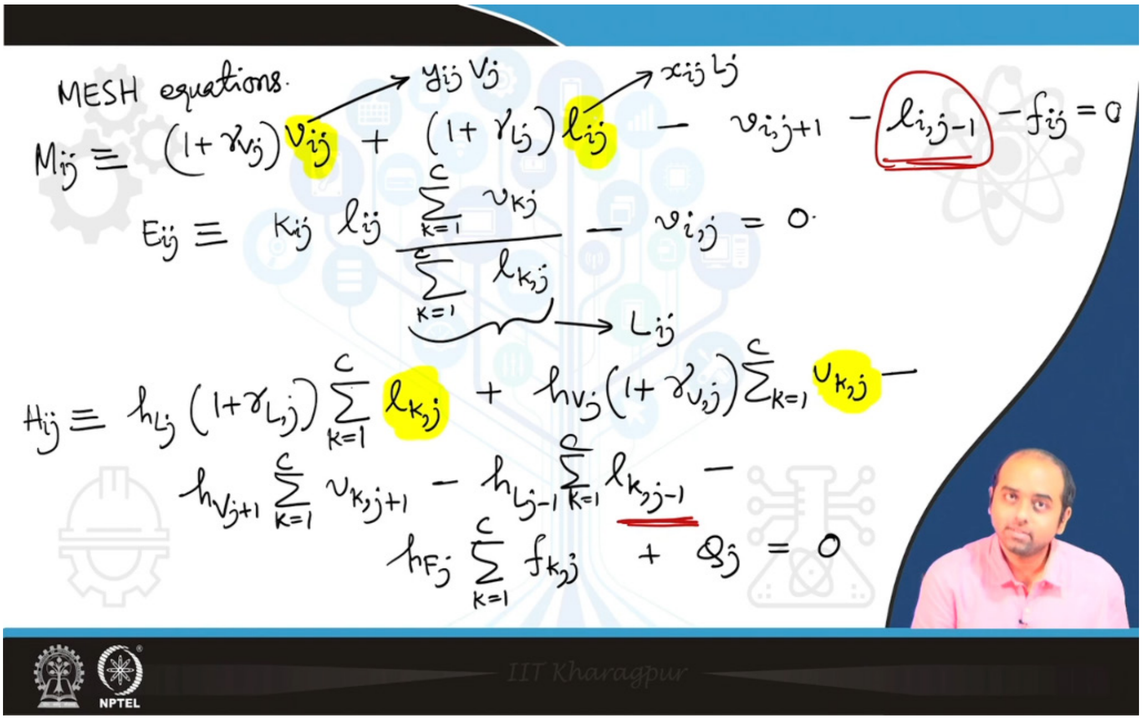

Similarly, if you work out the, try to understand the B j matrix, let me also try to write it down this B j which is d F j d X j. And I try to create the same structure starting from h j then we have M 1 j all the way up to M C j and then I have E 1 j all the way up to E C j. Here I will be having V 1 j all the way up to V C j T j L 1 j all the way up to L c j.

And if you observe carefully that here, since this is with respect to, it is j and not j minus 1 or j plus 1, for the h j equation there are terms representing V j in the h i j equation, you see that there are terms which represent this equation, V j is there. And also you have L j is also there. And this whatever h L j h V j all their function of T j.

So, essentially you will be having the first structure all the, I mean the first row all these values will exist. And for the M i j equations you see that you are having this V i j, you are also having the L i j. So, these components would exist. So, there is no possibility of M i j with respect to T i j. So, that will be zero. So, here in this general structure, you will be having all the diagonal elements to be existing.

And here also all the diagonal elements will exist because that derivative is possible. With respect to E i j, please, note that since it is a summation term, so, all the terms, I mean, this K j from 1 to K j all the terms would be there. Similarly, for L also all the terms from 1 to, sorry, not from 1 to C would be there. So, all these terms here for the M equation would exist. Rest would be zero.

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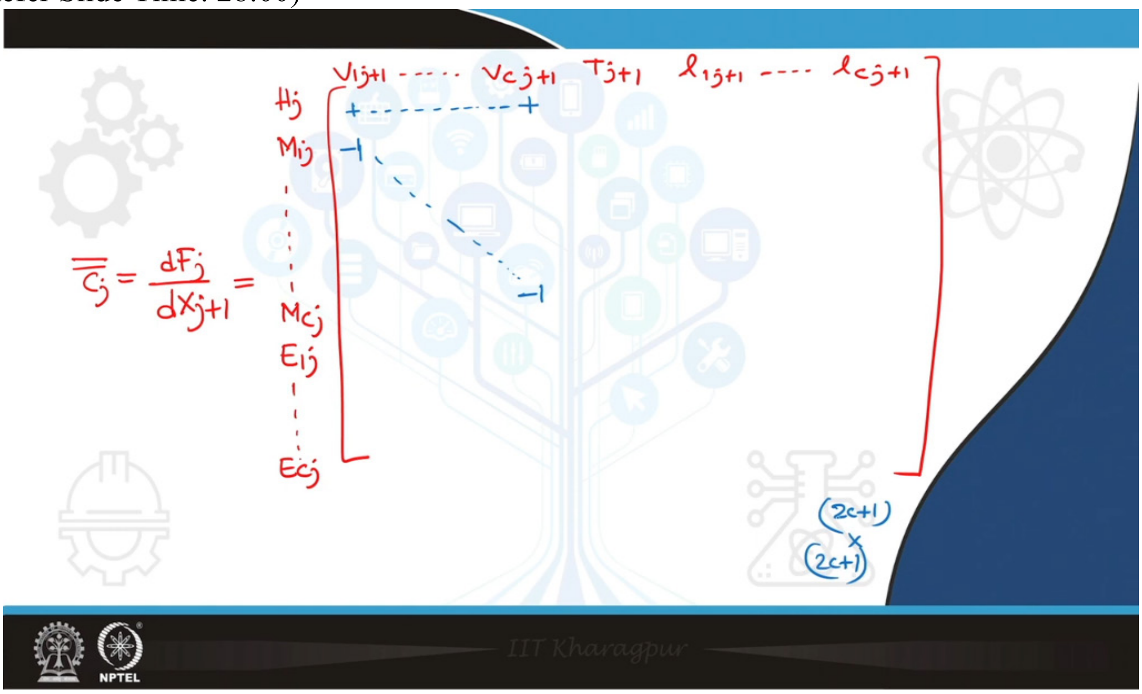

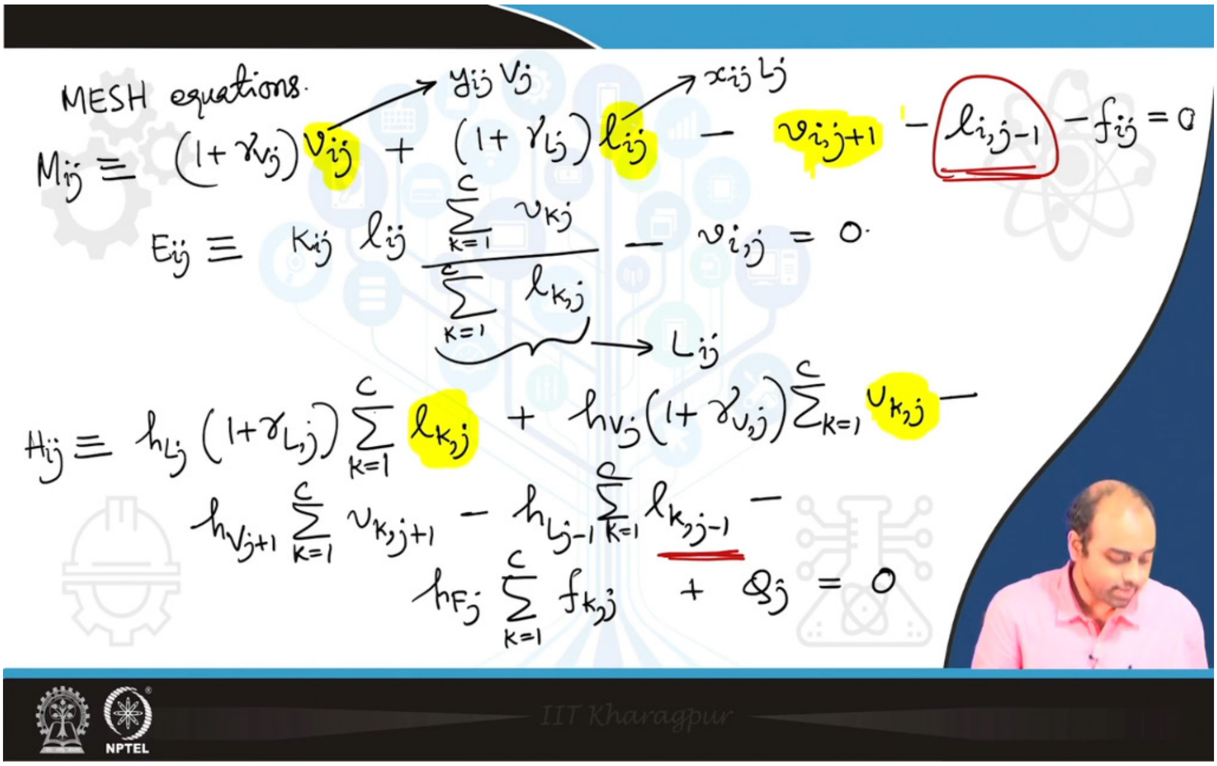

Similarly, for the C j matrix, let us try to get an idea of the how the structure will look like. C j matrix. So, that is d F d X d F j d X j plus 1. So, if I try to write down the different and in the top I write V 1 j plus 1 all the way up to V C j plus 1 then you have T j plus 1 L 1 j plus 1 all the way up to L C j Plus 1. And if you look carefully,

If you observe carefully, the enthalpy equations, let us go back and try to look into the enthalpy equations. So, if you see the enthalpy equations you have this j plus 1 term. So, that will exist. There is no L j plus 1 term and for the temperature h V j plus 1 is there. So, that temperature will exist.

As far as the M equation or the mass equation, you have the V j plus 1 term there for the M equations. This is the V j plus 1 term that you have and the coefficient is minus 1. And rest there is no L j plus 1 term, T j also does not exist. As far as the E i j is concerned, there is no j plus 1 term which exists. Similarly, there is no L j plus 1 term that is existing. So, matrix C and matrix A are more or less to some extent similar.

And so, these are the terms which will exist and these are the terms which will exist. In fact, this would be ideally minus 1 because we know that coefficient. And rest should be zero. So, this is again 2 C plus 1 cross 2 C plus 1 number of elements present in the C matrix. So, these all these A B C matrix will ultimately from the block tridiagonal matrix.

So, I hope all of you realize how to work out this calculation now. So, here the algorithm is very straightforward. That the essential idea is to first guess all the values of your T and j and then work out the individual component flow rates. Prepare the vectors and frame the block triadagonal matrix, evaluate the individual components, individual matrix of this block tridiagonal matrix and then feed the big matrix together.

And again, the idea of solving out the block tridiagonal matrix is same. But essentially, here you need to work out this what is the value of this inverse of the block tridiagonal matrix, for that you will once again use the Thomos algorithm and it is very same. So, instead of using for individual component here you will be applying that over small blocks in the block tridiagonal matrix where individually they are additional matrices.

So, I hope all of you get a nice overview on this 'simultaneous correction method'. Since, this is slightly more complex and the calculations are bit rigorous or long in terms of framing the block triangular matrix, so, we will not be doing any example problems on this case. But this is something you can definitely work out and if you want, we can also have small example on how to solve a block tridiagonal matrix actually.

So, with this I think you can look into online resource or any textbooks where I will see that how you can solve this block tridiagonal matrix using this idea or the same idea of the Thomas algorithm applied to the case of the blocks. So, I think with this I will close it here. I hope all of you like this lecture.