Mass, Momentum and Energy Balances in Engineering Analysis
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Lecture – 19
Solution of Macroscopic Balance Equations (Contd.)

Welcome, in this lecture we shall be doing a few more problems using the root finding methods. But in this lecture we shall be looking into some problems which have a set of equations. And that I have also told you in the class also that when we have a set of coupled algebraic equations, how we deal with them. And we shall be talking about non-linear algebraic equations.

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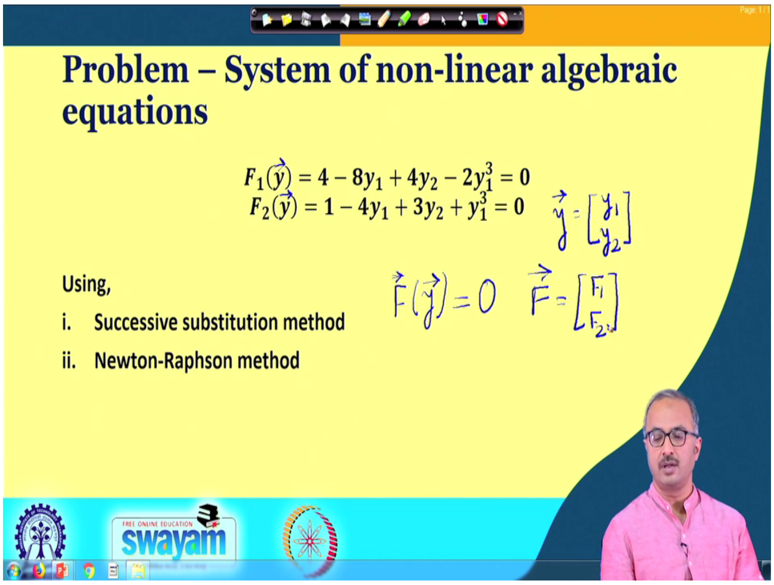

So, first we shall take an arbitrary problem here. So, I have not mentioned any kind of physical problem associated with this. But let me tell you that such kind of problems you often encounter whenever you are trying to have multi-dimensional flow or you have coupled momentum transfer, heat transfer, or momentum transfer, mass transfer, or coupled heat transfer and mass transfer. So, what happens in those cases that you write the balanced equations for the momentum transfer, for mass transfer, and for heat transfer. And then you find that all these equations become coupled because in the for example, in the heat transfer you will find the velocity is coming and the velocity is obtained from the momentum transfer.

And again in momentum balance equation you may find the various properties which you are using they may be varying with the temperature. So, you need to know temperature at each time instant and those temperature should be obtained from the energy balance equation. In similar fashion you may also find some dependency of the momentum or the energy or enthalpy on the composition of the particular system. And in the composition itself again will be dependent on the velocity profile or the temperature profile in the system.

So, in this manner you find a coupling is generated between all the three types of transport phenomena. And on top of that you if we have some kind of reacting term which gives rise to some generation or consumption term you find that the problem becomes further complicated. So, instead of taking those real life problems what I have done is this that I have just demonstrated the use of our methods of finding the roots which we have done earlier for single equations for a multivariable system with this particular problem. And you can easily extended for any other kind of real life problems.

So, here we have just taken these two equations only. And whenever we have two equations it becomes like quite simple in terms of solution. But please understand that in real life you may be having more than two unknown variables. So, here we have these two methods to be used here. And let me tell you that here we have shown this to F1 and F2 and these two y should be the vectors they are vectors; because this y vector is nothing, but the vector of the y 1 and y 2 so this is basically a vectors. So, if you put these two equations together it will be another vector F, another vector F which is the function of y vector and this is basically you are trying to solve it to be 0. And F is equal to this F 1 and F 2 vectors ok. So, that is how we look at this particular problem.

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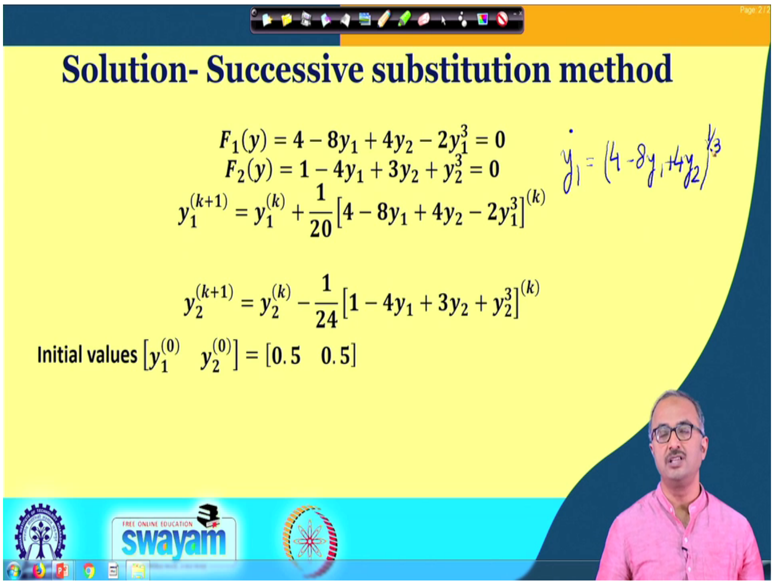

Now, first we try to implement this successive substitution method for this system of equations. So, here we write that we have to first find out the values of this y 1 y 2 from these two equations. And please always read this y as y vector; I am not putting the arrow all the times over this particular y ok.

Now, we can use any of these two equations to generate an appropriate expression in terms for y 1 and y 2. Here I have shown one way of finding it out you can have your other way. Like here we are taking from this particular equation we are finding the value of y 1 and from this equation we are finding the value of y 2 ok. So, you may try some other way that you may find y 1 here you have at what we are doing that y 1 we have taken with this particular expression and y 2 from this expression.

Another way that you can also take it to be a cube root if you take this particular term on the right hand side then you can easily see that y 1 may be taken as this particular this terms divided by 2 and cube root of that ok. So, that may be another way of finding this y 1 I am just writing for you here; like I can take y 1 to be 4 minus 8 y 1 plus 4 y 2 and cubic root ok.

So, this may be the expression for y 1 or you may even use this particular expression to get the value of y 1 ok. So, you have many choices to for this y 1 and y 2 for your understanding I have just taken 1 of the choices. So, here we have for y 2 and what we are doing now because this method need some initial guess values for bracketing the route. So, let us assume that y 1 0 and y 2 0 are like this ok. So, please understand that we have to bracket with respect to both y 1 and y 2 ok.

So, what we do here? So, we take this particular problem in this problem we choose these two equations for demonstration purpose. Now please understand that whenever when we have only two unlock the things becomes much simpler to find out to find the value of these roots. And understand this in this case is this y is basically a vector.

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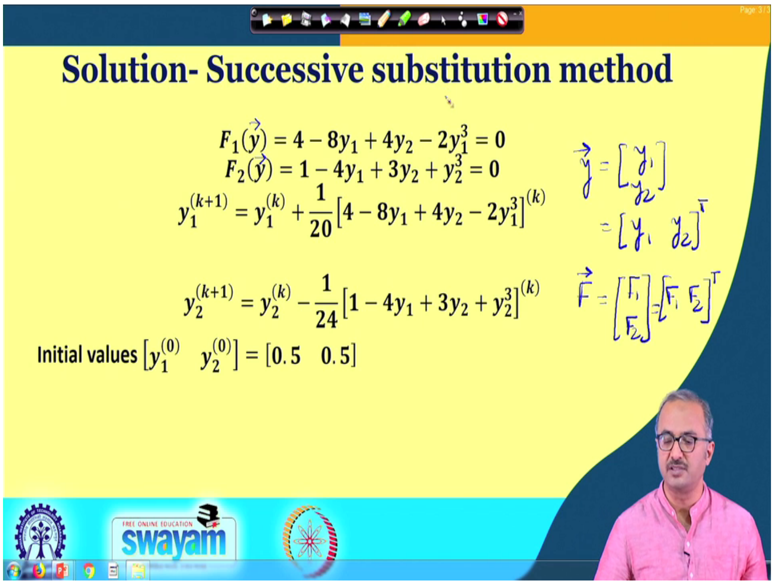

And this y vector is given by y 1 y 2 or is something it can also be written like y 1 y 2 transpose ok. So, this t is a transpose similarly this F 1 F 2 vector may be written like this that I can define another vector is that will be equal to F 1 F 2 or same as F 1 F 2 transpose ok.

So, these are various representation of these vectors and from now on I won’t be writing y with the particular arrow we shall understand by default that we are talking of a vector y. Now coming back to the problem in this problem we find that we have we have two unknowns y 1 y 2 and for this particular method what we need to do is this we have to represent y 1 and y 2 from these two expressions.

So, for example, I have taken these two expressions for y 1 and y 2 I have found the y 1 for the first expression and y 2 from the second expression; for your convenience I am giving you another option of choosing the y 1.

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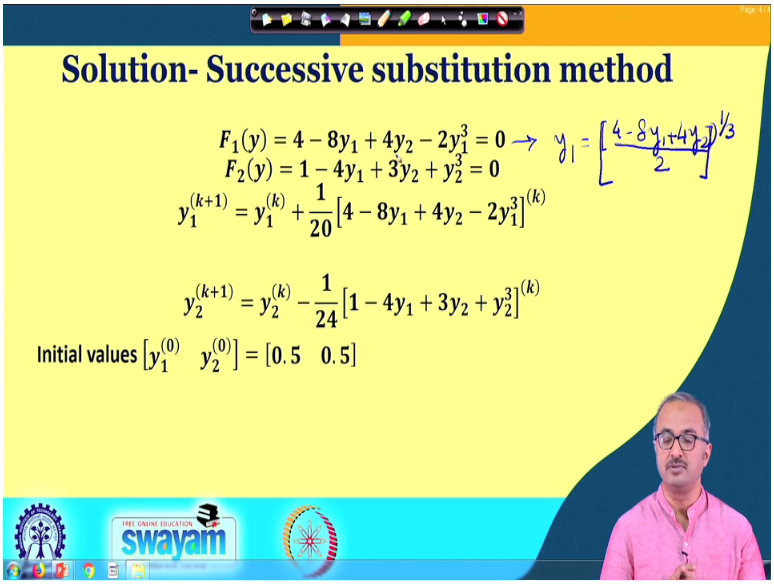

Like from this equation I can choose the y 1 like this; that means, I take the cubic root. So, this may be another way of representing the y 1. And similarly you can do the similar thing for y 2 form for this expression also you may get y 1 from this equation and y 2 from this equation. So, there may be multiple ways of choosing the expression for y 1 and y 2 from given set of equations.

And in my lecture I am also given some condition so that we are going to have convergence. So, that we do not have the instability problems in the solution. And with this particular given choice of y 1 and y 2 what we are going to demonstrate is that how we can proceed with the solution. So, as we have understood that for this particular method we need some initial choices of y 1 y 2. So, here we are using this two values right 0.5 0.5 for both the unknown variables.

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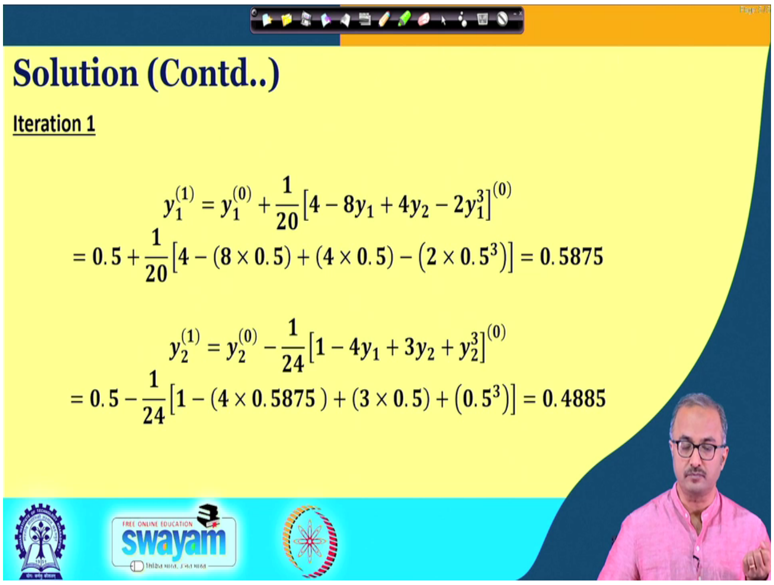

Now, what we do? We take the first equation the expression to update the value of y 1 and we just plug in the value of y 0 this shows that we are putting all this inside whatever is there inside the bracket at the 0th level. So, we put the 0th level values over here and update the y 1 value to this value. So, we can see that 0.5 it has moved up to 0.5875.

And next we what we do for y 2 also we update it and what we find that you are taking 0.4885. Now, please understand that depending on which expression you are taking this direction of the movement of these routes will also change. Now after this we can now move on to the second iteration.

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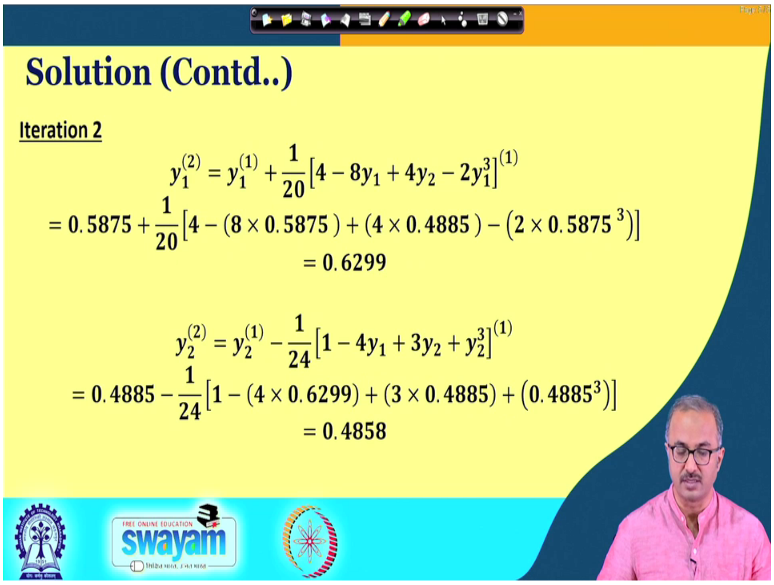

What we are now do we take the updated value of y 1 and y 2 and we again find updated value of the y 1 and now it is coming to 0.6299. And similar thing we do for y 2 and we find it is coming to 0.4858 it seems that if you look at these two expressions it seems that for y 2 with this particular choice we are able to convert faster than for y 1. And it is very much possible that different routes will convert at different rates to the solution and then whenever you are checking for convergence you have to take for convergence for each of the roots separately.

And whatever convergence criteria you may evolve that must take care that all the deviations for all the roots are taken care of and the precession and the accuracy must be ensured for all the roots involved in the given system of equations for a given process. So, here you can see that the route for y 1 with this particular representation is not converging so fast as it for y 2.

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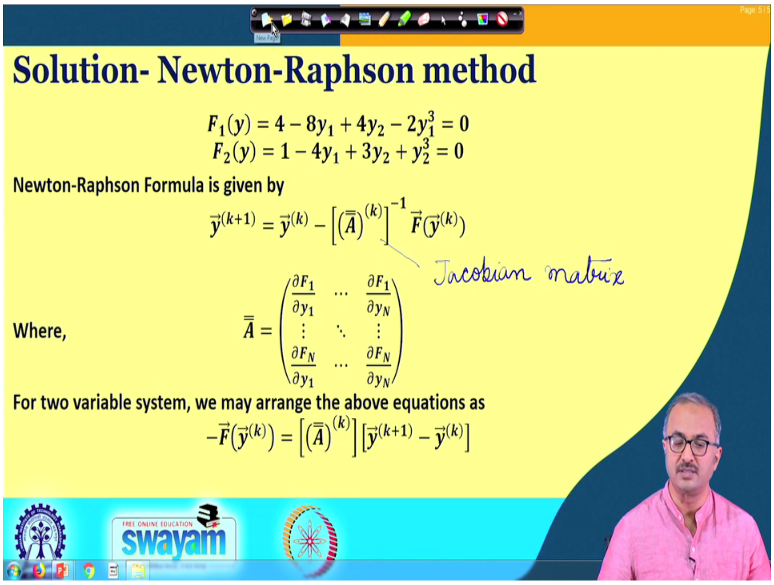

Now, you can keep doing these particular process and till you reach this convergence. Next we come to the implementation of Newton Raphson method for the same set of equations you may also wonder that why I am skipping for the second order Regular-Falsi method please understand that those may also be implemented, but their implementation becomes a bit more involved. So, that for multi component system or whenever we have multivariable systems we generally do not adopt those Regular-Falsi and secant method.

We rather go with these 2 methods which I have demonstrated in this particular lecture and now we go to the Newton Raphson method. And as I showed you in my lecture in this case the y will be obtained by this that we have a particular Jacobian for your recollection I just write that this is the Jacobian matrix. And this is the matrix of the partial derivatives ok. So, we need the Jacobian in whenever we have multivariable problem for Newton Raphson method and then what we do that we find this Jacobian from this expression; that means, we have to take the partial derivative of all the functions with respect to each of the unknown variables.

So, in this case we have two unknown variables and two functions. So, this will be reducing to dou F 1 by dou y 1 dou F 1 by dou y 2 and dou F 2 by dou y 1 and dou F 2 by dou y 2 so; that means, it is giving rise to A 2 by 2 matrix ok. And then we have to take the inverse of this particular Jacobian matrix multiplied with the this function vector at which is evaluated at the present level of iteration with the present values of the unknown variables and so that we get the updated values ok. So, this is a two variable problem so for which I have just shown you how we can simplify this solution. So, whenever you have this two variable problem you made do this that you can rearrange the address the equation; so, that you can avoid the evaluation of the inverse of a matrix. Please understand window systems becomes larger we cannot do this kind of an rearrangements and we have to have the matrix inversion of in the particular computation.

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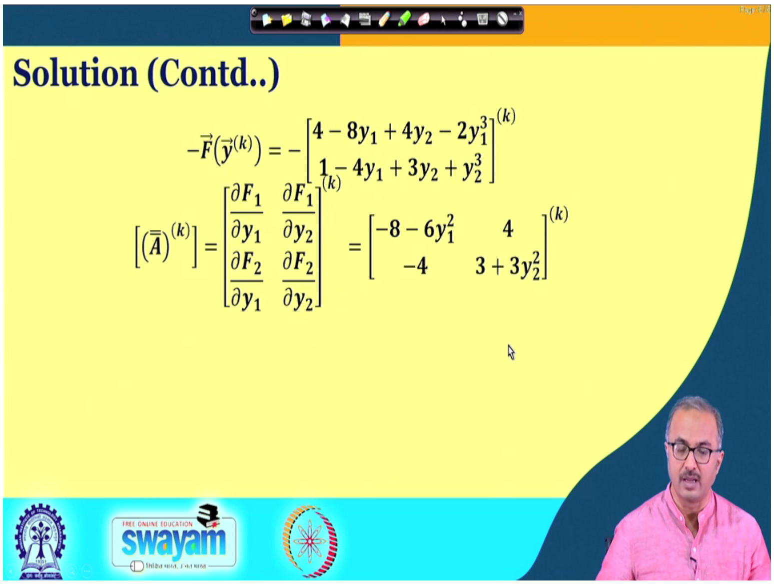

So, let us do this that we arrange it and we get this particular Jacobian matrix. Now this is a function matrix and the Jacobian matrix as I told you. So, if you take the derivative with respect to y 1 and y 2 for both the functions we obtain this as a Jacobian ok. So, this is the vector of the functions.

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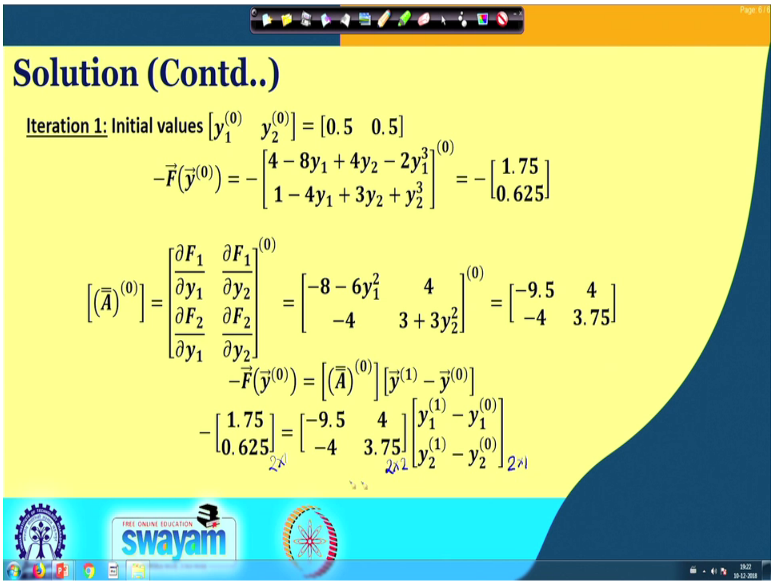

Now, let us have this initial guess values as 0.5 0.5 as we have done for the previous way of solution by the successive substitution. So, here what we do we evaluate the function values at this base values has used and then we also evaluate the Jacobian matrix ok. And we put these values and we get this particular Jacobian and now what we do is simply plug-in the values over here and we get this kind of a matrix instance and you can easily see that from your linear algebra you know this is 2 by 1 this is 2 by 2 and this is 2 by 1. So, that is resulting this resulting product will be having a dimension of 2 by 1. So, this is a kind of internal check for you that you are in the right path.

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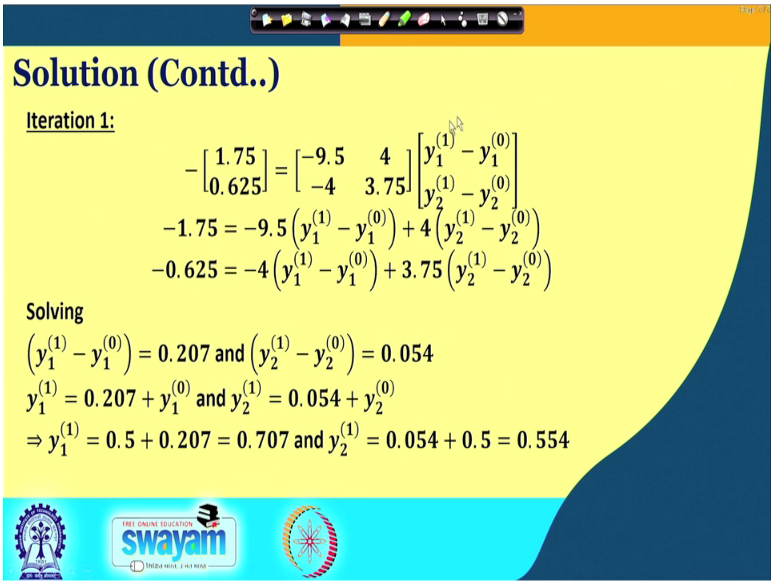

So, in the first titration what we do we simply multi apply this matrix with a vector and b gain this expression and this expression. Now you can see that we have to unknown and two linear algebraic equations and for because it is any two variable we can easily find out the values of these two unknowns by rearrangement. And we can see that I am not going to details of this evaluation of this y 1 y 2 values you know it quite we will. So, see that we are getting the value of y 1 and y 2 like this ok. So, after getting these values we can see that 0.5 we have moved up to 0.7 and for y 1 and we have move up to 0.554 for y 2.

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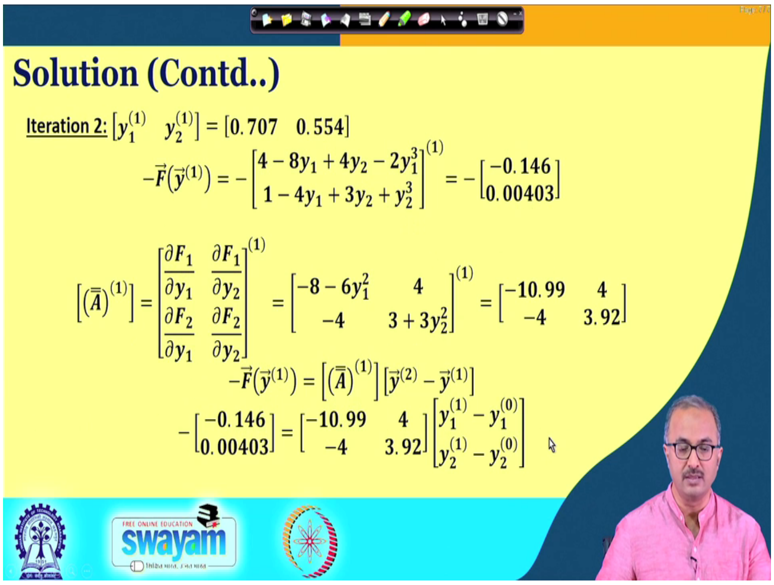

Now, taking these values of y 1 and y 2 we again go for the next iteration. Here again we find out the function values over here and the Jacobian we are evaluate for the new state of y 1 y 2 here we get them. And again we put these values over here in this equation.

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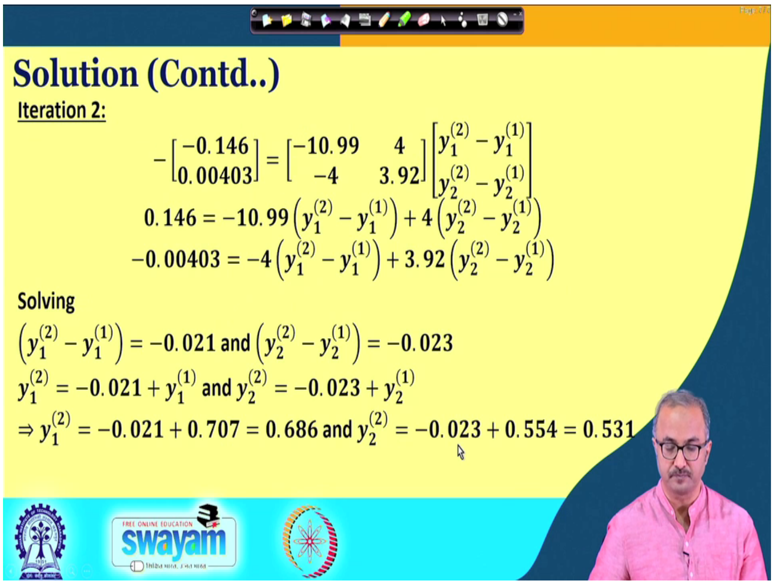

Again we obtain a set of two linear algebraic equations; from these two equations we can find out the value of the y 1 and y 2. Again you can see here that because Newton Raphson is quite effective if we are nearby the route we can see that the way these two values are trying to get converged. So, this you can carry forth and to get the actual solution.

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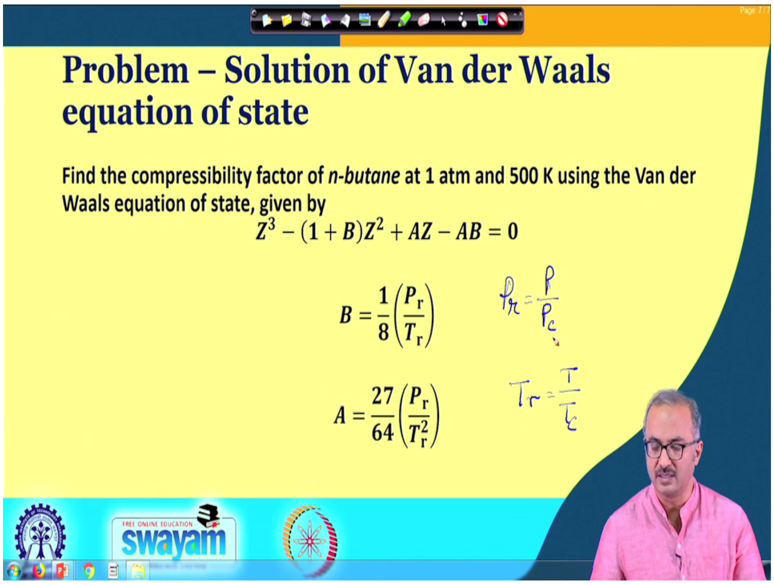

Now, we come to the solution of an equation of state. This I told you separately because in this cubic equation of state we have to find out three values of either the compressibility factor or the volume ok. So, depending on the way we are rearranging the equations. And as I told you in the class that there are many cubic equations of state like Van der Waals is the first one and then we have Peng – Robinson equation we have (Refer Time: 18:59) equation so on and so forth. So, for your understanding and for demonstration purpose we have taken a Van der Waals equation of state, but this is not restricted for this particular equation of state.

So, here we have review to find out the compressibility factor for n butane at 1 atmosphere and 500 K using the Van der Waals equation of state. Now, please understand that this even though this particular problem is asking us to find out the value of Z, but these Z value may also be used to find o ut the density of the particular fluid ok. So, we may not stop at Z. So, for demonstration purpose we are stopping at Z. So, if you go to the Van der Waals equation of state you will find these are the values of the parameters involved in the equation.

And you see that these are given in terms of the reduced pressure and reduced temperature. And what are these are nothing, but the ratio of the actual value to the critical value; that means, if I want to find a reduced pressure this is equal to the actual pressure divided by the critical pressure. Similarly the reduced temperature is equal to the actual temperature divided by the critical temperature ok. And these critical values are dependent on the particular type of the species. So, we get the values of the critical values from the literature.

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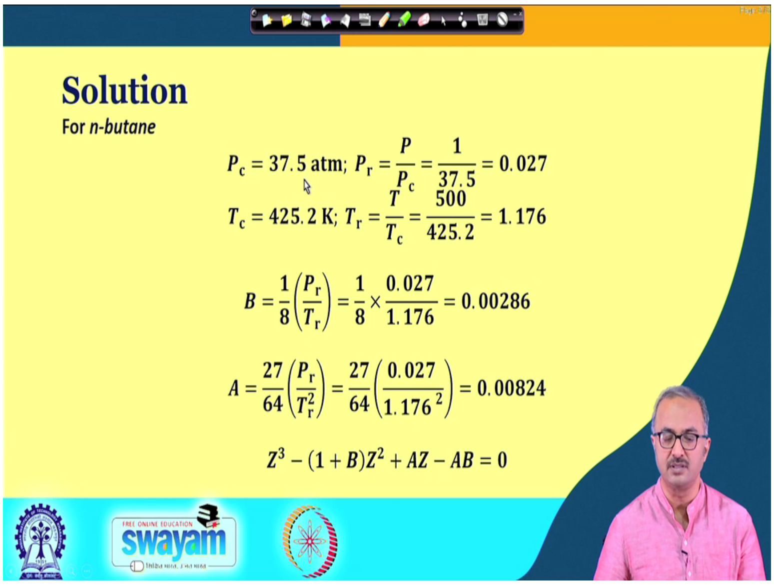

Now, we can proceed with the butane. So, here we have that for butane we have this is the critical pressure and is a critical temperature and we find out the reduced pressure and reduce temperature values here. And what we do when we find out the values of this particular coefficients ok. Now, once we find the coefficient we put these things in this particular expression.

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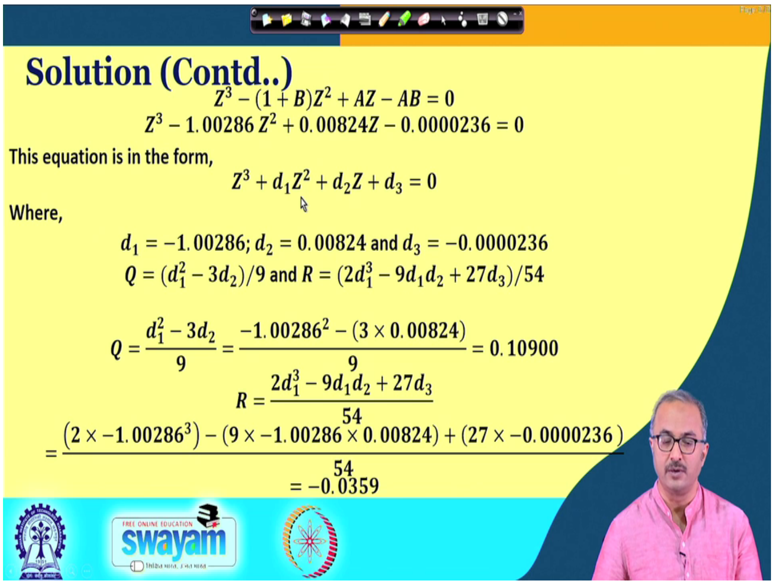

And we have finally, this expression. Now in the lecture what I showed you that we have this form of the equation based on this form of the equation we use the Cardano's method to find out the values of the z these values of the z. So, please understand these values of the z may be positive negative or even imaginary ok.

Now, as I explained in that vector that we find the values of d one d two and d three and then these two more parameter based on this d 1 d 2. So, here we see the by comparison we see that the d 1 is minus 1.00286 and d 2 is plus 0.00824 and d 3 is minus 0000236. And we find the values of this Q and the R from these two expressions ok. So, we find these values of R and Q and then what we do.

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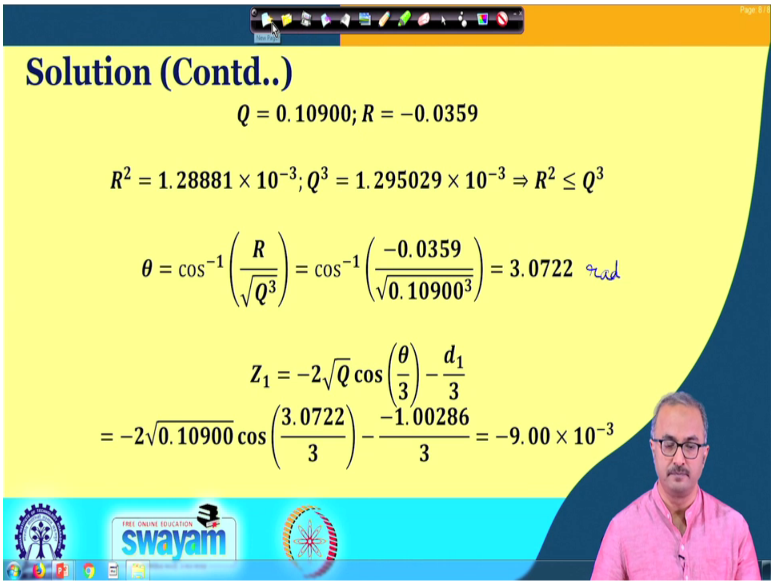

We find out the values of R square and Q cube. And we find that R square is means satisfying the condition that it is less than the Q cube as given by Cardano. So, in that case these are the solution way that we have to find out that the value of the theta that is coming in terms of cos inverse of R by under root Q cube. So, we put the value of theta here and please understand this theta is in radian ok. So, we put this value of theta over here and it is in terms of radian. So, we put the value of theta over here we find the value of Z 1.

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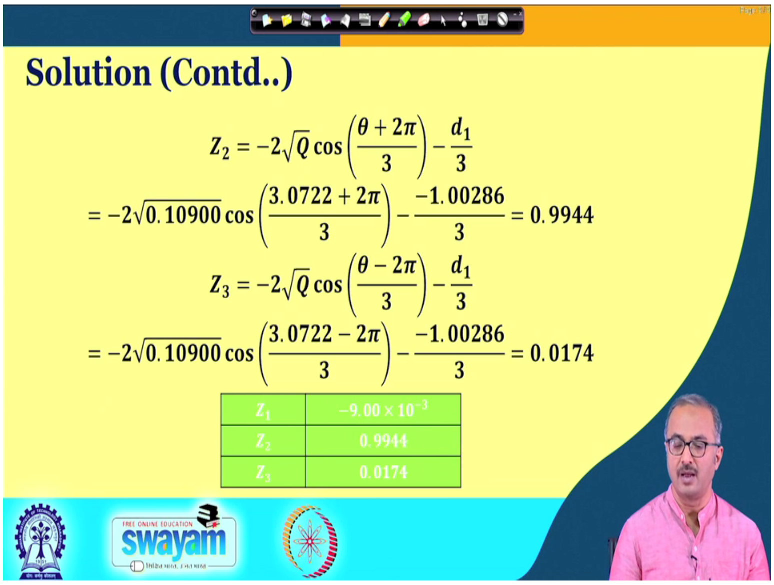

And then we find the value of Z 2 and Z 3 from the expressions given by Cardano. So, we find now summer them we find that we are getting this three values of the roots for the compressibility factor. So, one of them is coming to be negative and one of them is coming to be here 0.99 nearby 1. And one of them is coming to be quite low ok.

Now, you will see that if you go through the book for thermodynamics, you will find that how all these values of the compressibility factor are interpreted and that used. So, I am not going into those theories I am stopping at the finding of the routes for the compressibility factor by using a suitable numerical method. And also please understand there are many other methods which have been proposed to solve these cubic equations of state after Cardano.

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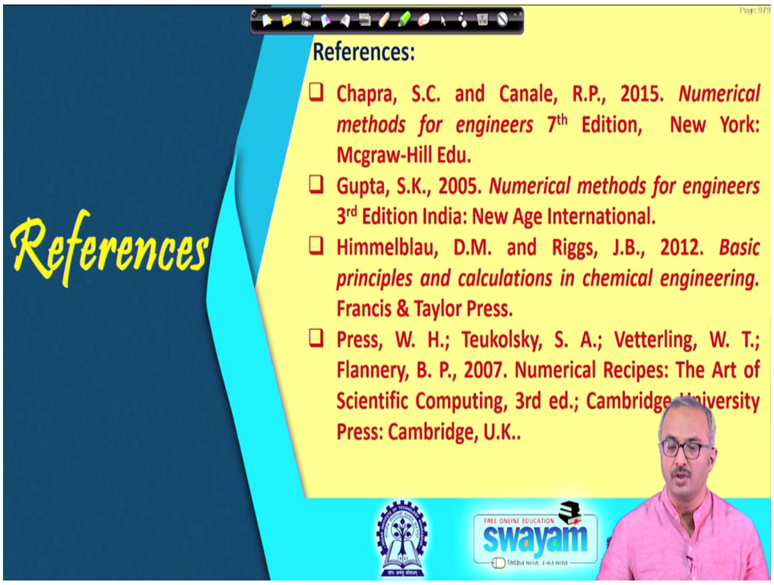

So, here we have a few selective references for more detail on these particular methods.

Thank you.