Advanced Mathematical Techniques in Chemical Engineering

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Module No. # 01

Lecture No. # 20

Special Function

Welcome to this session of our lecture. So, it is basically, if you remember whatever we have done in the last class, in the last class we were looking into the eigen values and eigen functions of the form of the equation d square y dx square plus lambda y is equal to 0.

So, we have already seen what will be the form of eigen values and eigen functions, if we have both boundaries the dirichlet boundary condition. Now, if we change the boundary condition at X is equal to 0 by a Neumann boundary condition then, we have also seen how the form of the boundary eigen values and eigen functions will take.

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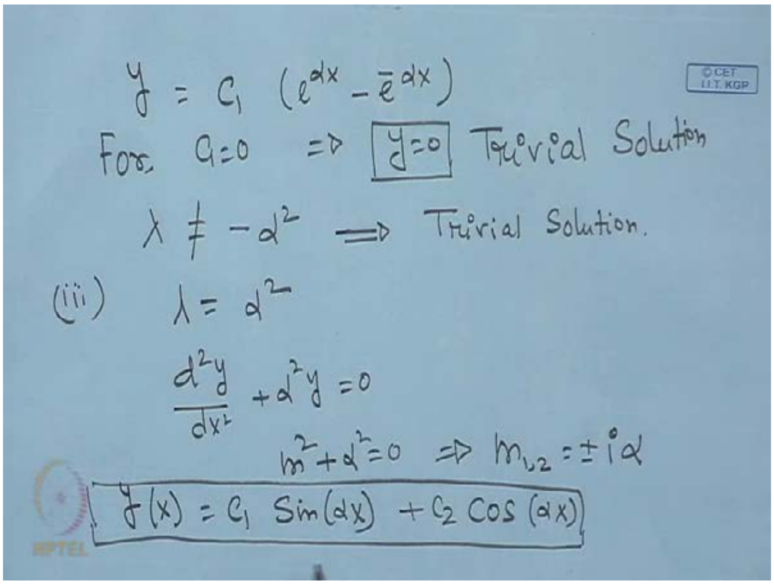

Now, in this third problem, we have taken up that we have changed the boundary condition from one of the boundary condition of dirichlet to a robin mixed boundary condition and we are looking into the eigen values and eigen functions for this particular case. And we have already seen that, the lambda cannot be 0, if lambda is equal to 0, then we are going to get a trivial solution. If lambda cannot be negative, if lambda is negative then again, we are also going to get a trivial solution. So, therefore, the only option that is left is lambda is positive and lambda is equal to alpha square, so you will be having d square y dx square plus alpha square y is equal to 0.

Now, we have already seen that, the form of the equation will be e to the power mx, so you will be getting m square plus alpha square is equal to 0 and you will be getting m 1 2 as plus minus i alpha, so the solution of this equation is a combination of the periodic functions, sine functions and cosine functions.

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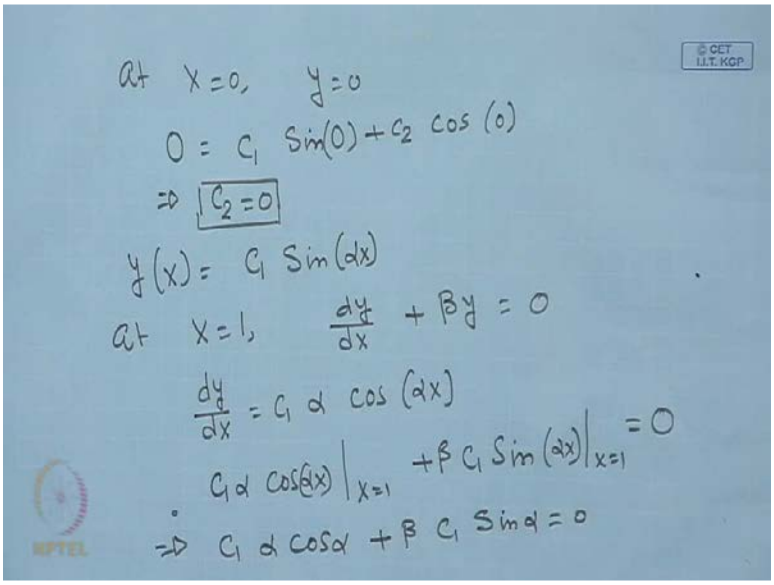

So, y is equal to c 1 sine alpha x plus c 2 cosine alpha x is the solution to this problem. Now, we apply both the boundary conditions to evaluate the constants c 1 and c 2. So, if we do that, the first boundary condition is at x is equal to 0, y is equal to 0, so what we get is that 0 is equal to c 1 sine 0 plus c 2 cos 0.

So, sine 0 is 0, cos 0 is 1 so therefore, we will be getting here c 2 is equal to 0, so what is the solution? The solution is of course y is equal to 0 is equal to c 1 sine alpha x, so c 1 sine alpha x is the solution. Now, let us utilize the other boundary condition and see what information we can extract for the corresponding to evaluate the value of alpha.

So, if you look into, if you remember the other boundary condition at x is equal to 1, dy dx plus beta y is equal to 0, so we evaluate dy dx from here, so dy dx is nothing but c 1 alpha cosine alpha x and y is c 1 sine alpha x. Now, we put these things, we evaluate this quantities at x is equal to 1 and put it here, so dy dx is c 1 alpha cosine alpha x evaluated at x is equal to 1 plus beta times y is c 1 sine alpha x evaluated at x is equal to 1 is equal to 0, so c 1 alpha cos alpha plus beta c 1 sine alpha is equal to 0.

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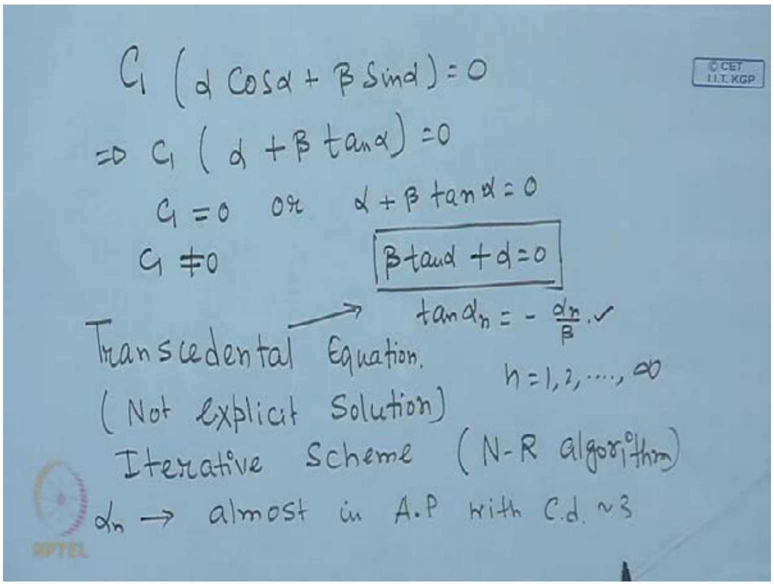

So, we get these equation from using this boundary condition and see what we get we just take c 1 common, if we can take c 1 common, it will be alpha cosine alpha plus beta sine alpha is equal to 0. So, you divide both the both side by cosine alpha, we will be getting alpha plus beta tan alpha is equal to 0. Now, there are two options again in this case to satisfy this equation, first one is c 1 is equal to 0 or the quantity in the bracket is equal to 0, alpha plus beta tan alpha is equal to 0.

Now, if c 1 is equal to 0 again, we are going to get a trivial solution because the solution if you remember, it is in the form of y is equal to c 1 sine alpha x. So, therefore, c 1 cannot be is equal to 0, because if c 1 equal to 0, we are going to get a trivial solution; so what is the option now left, beta tan alpha minus plus alpha is equal to 0.

Now again, this is a transcendental equation, there are n number of roots of tan alpha is equal to minus alpha n by beta, so this is known as a transcendental equation. Now, unlike the previous two cases, we had explicit solution for alpha n, but in this case, you would not be getting an explicit solution of our alpha n, we will be getting a transcendental equation in this form.

Now again this equation, tan alpha is equal to minus alpha by beta will be having n number of roots depending on the value of beta. So, depending on the value of beta, it will be having n number of roots and this value the index n runs from 1, 2, 3 up to infinity and since we are not getting an explicit solution of alpha n from this equation, unlike the previous two cases, this equation has to be solved numerically, so this is known as a transcendental equation, it is not explicit equation.

So it is implicit equation, not explicit solution. So, we have to solve this equation numerically in order to or we have to take up take any iterative scheme for solution of this equation, tan alpha n is equal to minus alpha n by beta. We can talk about a Newton Raphson algorithm and solve this equation, now if you put different values of beta, typically these roots, this will be having the solutions of alpha n will be in the they will be increasing they will be almost arithmetic progression with a common difference of about 3.

The nature of this equation is such that, this alpha n will be having will be they are almost in arithmetic progression with a common difference about 3. So, there is a trick to solve this equation by using Newton Raphson technique, the trick is that, you take depending on the value of beta, we have to put the value of beta and then you have to give a guess value of alpha.

So once we know the beta, beta is nothing but a system parameter knowing the value of beta, we give a guess value of alpha, the first root will be converging that will be giving you the value of alpha. The next you give a guess which will be nothing but, the earlier solution plus 3 so you with that guess, you put a you will be getting the next root of this transcendental equation and once you do that, then you give the third guess as the solution of the second loop second eigenvalue and then plus 3, the common difference is plus 3.

So, the whole numerical algorithm will be put into two loops, the internal loop will be the Newton Raphson rule loop for a known value of beta, the outer loop will be consisting of 3 values, will be consisting of the guess value which will be given in the increment of alpha.

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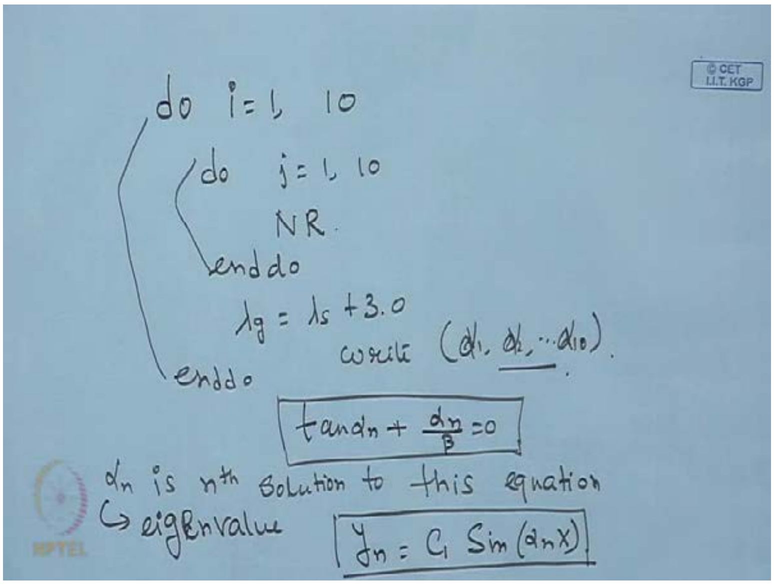

So, if we look into the structure of numerical solution, the structure will be there will be two loops, i is equal to 1 2 let us say 10, this will be computing the 10 eigenvalues, do j is equal to 1 to 10. So, first loop will be Newton Raphson for solution of this, so it will be we just finish it off here, then whatever the solution you are going to get, this lambda guess will be nothing but lambda solution of the earlier case plus 3.

So that ends the outer loop, so this will be the inner loop, this will be the outer loop and at the end, you are going to get all the solutions, eigen values lambda 1 lambda 2 up to lambda alpha 1 alpha 2 up to alpha 10.

So that is why that is how, one can compute the eigenvalues of this transcendental equation. So, what is the corresponding value, so we cannot get the explicit expression of the eigenvalues in this particular case. So, we write down this transcendental equation in order to designate this eigen value, alpha n divided by beta is equal to 0. So, we say alpha n is the solution is the n th solution to this equation, this also known as n th 0 to this equation.

So, these are the eigen values n th eigen, so alpha n is the n th eigen value, which is nothing but the n th solution to this equation. And what are the corresponding eigen functions? The corresponding eigen functions will be c n c1 sine alpha n x, so n th eigen functions is c n y n is equal to c 1 sine alpha n x.

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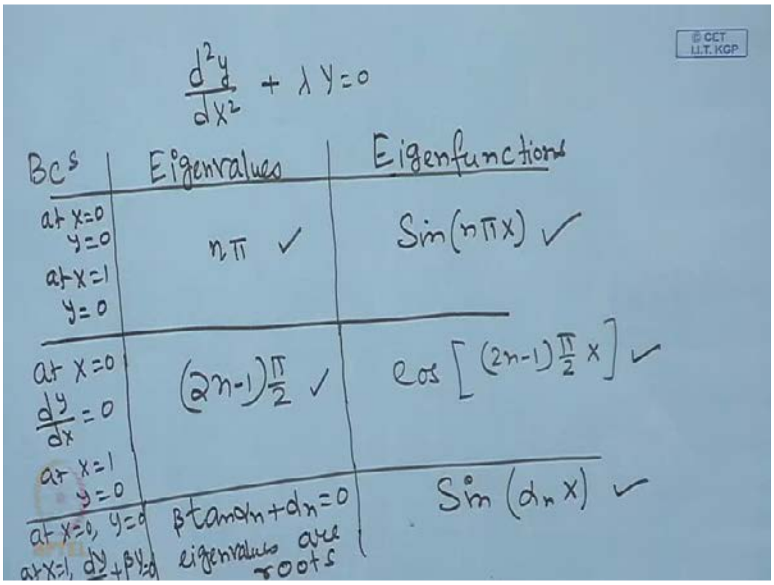

Now, let us summarize what we did. We looked into the solution to this, we looked into the non-trivial solution to the equation d square y dx square plus lambda y is equal to 0 and we use the following boundary conditions and see what are the eigenvalues we got and what are the eigen functions we got. So, these are the boundary conditions and these are the eigenvalues and these are the eigen functions. So boundary condition, the first boundary condition is that, at x is equal to 0, y is equal to 0, at x is equal to 1, y is equal to 0.

So with this, we got the eigenvalues as n pi and the corresponding eigen functions are sine functions, sine n pi x. If we had the boundary condition at x is equal to 0, a Neumann one so it becomes dy dx is equal to 0 and at x is equal to 1 y is equal to 0, we have 2 n minus 1 pi by 2 as the eigenvalues and cosine functions as eigen functions. And on the other hand, the last one if we have the boundary condition at x is equal to 0, y is equal to 0 but at x equal to 1, we have a robin mixed boundary condition dy dx plus beta y is equal to 0.

Then we have a transcendental equation, which is the solution of this transcendental equation becomes eigen values, so beta tan alpha n plus alpha n is equal to 0. So, eigen values are roots of this equation or zeros of this equation and the corresponding eigen functions are sine alpha n x.

So if you see, if we just change the boundary conditions, the eigen values and eigen functions change, if we have dirichlet boundary conditions on both the boundaries, the eigen values are n pi and eigen functions are sine functions.

If we have a Neumann boundary condition at x is equal to 0 and dirichlet boundary condition at x is equal to 1, we have 2 n minus 1 pi by 2 as the eigen values and cosine functions as eigen functions. Similarly, if you have dirichlet boundary conditions at x is equal to 0 and a robin mixed boundary condition at x is equal to 1, we will be having a transcendental equation, roots of whose are at the solutions or the eigenvalues of the problem and sine functions are the eigen functions.

So we have seen that, for by selection of different boundary conditions, one can get into you can land up into the different eigen values and eigen functions. In most of the chemical engineering applications, these are the boundary conditions and we are dealing with and these are the eigenvalues and depending on the boundary conditions and situations, one can land up with different eigen values and different eigen functions.

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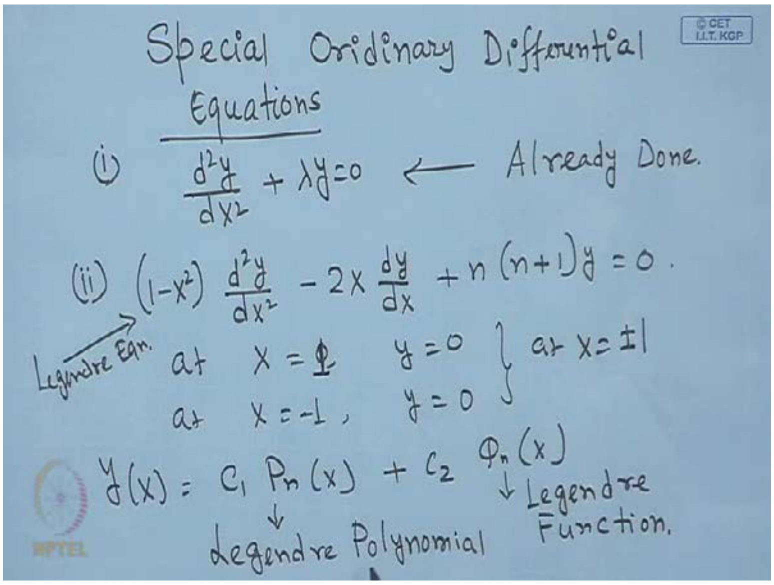

So next, we will be looking into some of the special ordinary differential equations which are in the for which, the eigen values and eigen functions will be defined. The first case we have taken, that is not a special one, that is the that is in cartesian coordinate d square y dx square plus lambda y is equal to 0, we have already taken care of this equation, this we have already done.

Next special ordinary differential equation, we will be looking is this form 1 minus x square d square y dx square minus 2 X dy dx plus n to n plus 1 into y is equal to 0. The boundary conditions are at x is equal to 0, y is equal to 0, at x is equal to 1, x is equal to plus 1 y equal to 0, x equal to minus 1 y is also equal to 0.

So, this will be x equal to plus 1 this equal to x equal to minus 1; so this is basically at x is equal to plus minus 1. Now, again if you see that the differential equation is homogeneous, there is no non-homogeneity term is present there, the boundary conditions are also homogeneous.

So, therefore, this will be admitting, this will be giving, a this this will be a candidate this set of this system including the differential equation and the boundary conditions is a candidate to have a eigen value problem. So the solution of this equation is in the form of c 1 P n x plus c 2 Q n x, where P n is known as the Legendre polynomial and Q n is known as the Legendre function.

If so we have already seen that, if this is the form of the in the first case, this is form of differential equation, the sine function, cosine function etcetera, the eigen functions and we have already seen the eigen values, but if the form of the equation is a special equation like this, this is known as the Legendre equation. And this occurs mostly in spherical polar coordinate system, then if this is the govern, this is the differential equation with this homogenous boundary condition that at x equal to plus minus 1, it is equal to 0, then the solution will be constructed by combination of Legendre polynomial and Legendre function.

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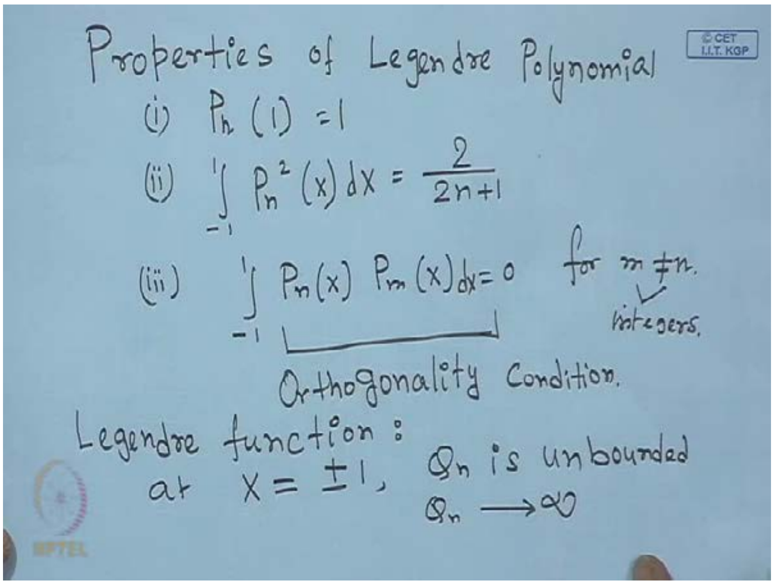

Then we should know about some of the properties of this Legendre polynomial or Legendre functions, so we list down some of the important properties of Legendre polynomial. This one or first one is P n of 1 is 1, so that is the first property, second one will be minus 1 to plus 1 P n square x dx will be 2 divide by 2 n plus 1 and third one will be minus 1 to plus 1 that is a domain of x P n x times P m x is equal to 0, for m not equal n, where m, n are integers.

So, this is also known as the orthogonal property, if you remember the inner product as we have defined earlier for 2 matrices, for two vectors, we have found out the inner product between the two vectors will be equal to 0 and in case of continuous domain, in case of continuous function, inner product is nothing by it will be replaced by an integration, so integration of P n x multiplied by P m x dx will be equal to 0.

So, therefore, this is also known as the orthogonality condition. Now, let us look into the sum of the property of Legendre function. So, these are the most important properties which will be utilizing quite often, whenever will be talking about a Legendre equation as our governing equation. For Legendre function, the property is that at x equal to plus minus 1, Q n is unbounded; that means Q n tends to infinity or it will be infinite in nature.

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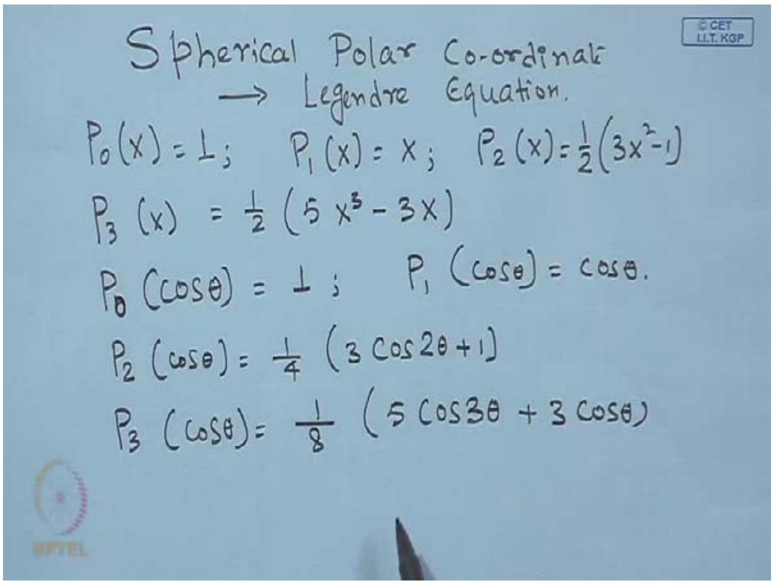

So, that is the property of Legendre function, that is at x equal to plus minus 1, Q n is unbounded. Now typically, we will be dealing with the Legendre functions, Legendre polynomial and Legendre equation, whenever we are working on in spherical polar coordinate will be landing with the Legendre equation.

Now, some of the properties, some more properties that P 0 x is equal to 1, P 1 x is equal to x, P 2 x is equal to half 3 x square minus 1, P 3 x is half 5 x cube minus 3 x, P n cosine theta is 1 P 1 cosine theta is cosine theta, P 2 cosine theta is 1 by 4 3 cos 2 theta plus 1, p 3 cos theta is 1 over 8 5 cos 3 theta plus 3 cos theta, so this is P 0, this can be P m (Refer Slide time: 24: 44).

So, P 0 cosine theta, so these are in polar coordinate, we just replace x is equal to cosine theta, so we will be getting P 0 cosine theta is 1 P 1 x by cosine theta is cosine theta P 2 cosine theta is equal to half 3 cos square theta minus 1, that is given by 3 cos 2 theta plus 1 and similarly, we will be getting P 3 cosine theta.

So, in spherical polar coordinate, we will be getting the Legendre equation as your governing equation and the solution will be constituted by Legendre function and Legendre polynomial. We have discussed some of the properties of Legendre polynomial, Legendre function, the major property is that, it goes unbounded at the 2 boundaries x equal to plus minus 1.

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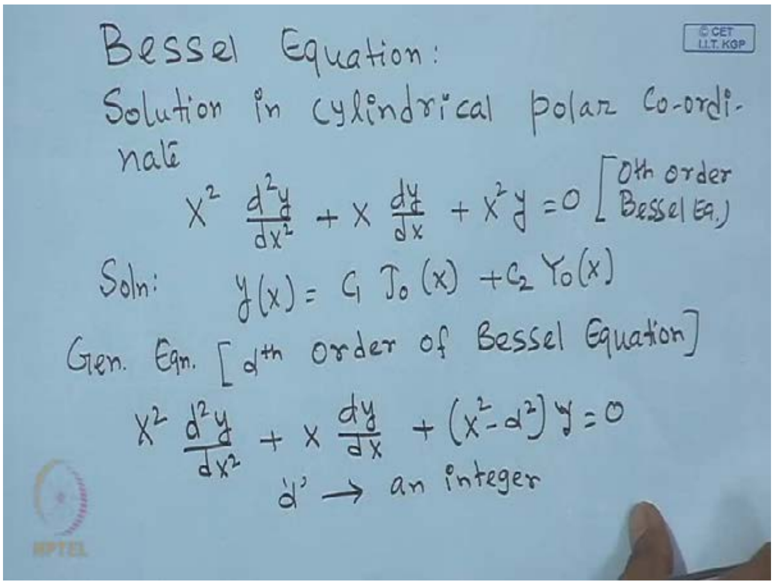

Next, we talk about a particular form of or a special form of ordinary differential equation that is a Bessel equation. This equation will be in common, whenever we are talking about the solution of solution in cylindrical polar coordinate, whenever we are working in cylindrical polar coordinate system, we are landing up with the Bessel equation. So, the Bessel equation is in the form of X square d square y dx square plus X dy dx plus X square y is equal to 0.

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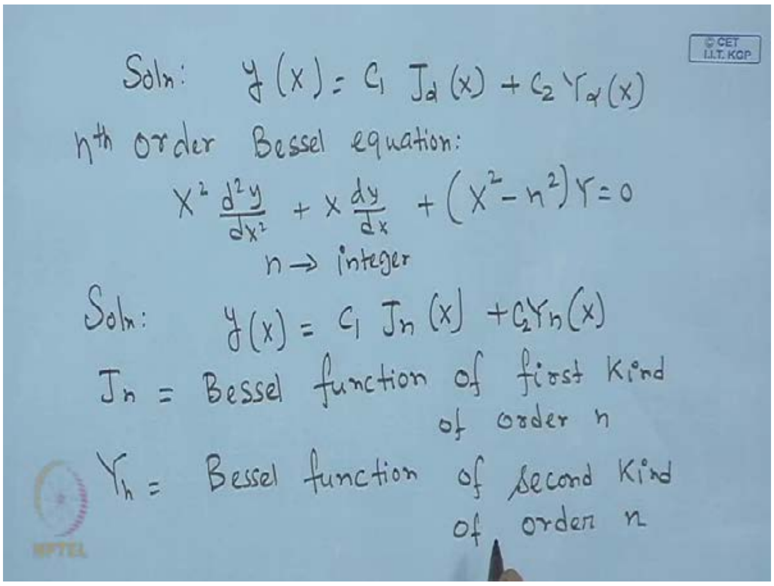

So, the solution of this equation is in the form of y of x is equal to c 1 J 0 x plus c 2 Y 0 x. For a general equation, this is known as zero th order Bessel equation, general equation means, it is alpha th order of Bessel equation and the equation is in the form of X square d square y dx square plus X dy dx plus X square minus alpha square times y is equal to 0, where alpha is an integer.

So, you just check if we put alpha is equal to 0, we are going to get back these equation, the zero th order Bessel equation for alpha is equal to 1, for any value of alpha, you will be getting this is the Bessel equation, for alpha is equal to 1, the last term will be X square minus 1. So, the solution of this equation is in the form of y x is equal to c 1 J alpha x plus c 2 Y alpha x, so you can replace alpha by n, so you will be getting nth order Bessel equation.

So, nth order Bessel equation is nothing but, X square d square y dx square plus X dy dx plus X square minus n square y is equal to 0, n being an integer, again the solution is composed of J n and Y n. So, c 1 J n x plus c 2 Y n x, so we will be having J n as the Bessel function of first kind of order n and Y n is the Bessel function of second kind of order n.

So now, these will be quite common, whenever we will be talking about the cylindrical polar coordinate system, the solution will be composed of Bessel functions, first kind and second kind. And then, let us look into some of the important properties of Bessel functions, which we should know and they are very important and they will be useful whenever we will be solving this type of equations.

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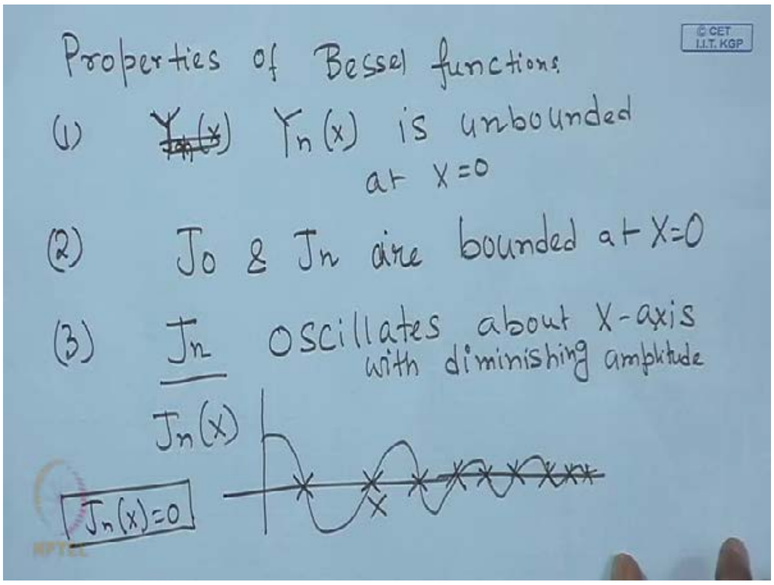

So properties of Bessel equations, Bessel functions, most important property is that y alpha x or Y n x the Bessel function of second kind of order n is unbounded at X is equal to 0, that means at X is equal to 0, Y n x goes to infinity irrespective of any value of n.

Second important is that J 0 and J n, for any n equal to 0, 1, 2, 3 is they are bounded at X is equal to 0, that is quite important; the third one is that J n oscillates about x-axis. So that means, this is very important property like the sine functions and cosine functions or the trigonometric functions like sine functions, cosine function, tan function they in fact tan functions they do not oscillates, but the sine function and cosine functions they oscillate about the x-axis. Similarly, J n oscillates about x-axis, so if we plot J n x as a function of X, it oscillates about x-axis with diminishing amplitude that is important.

So, therefore, J n x will cross the x-axis at several points and all these points are the roots of the equation are the eigenvalues of the corresponding problem. So, we can easily evaluate, so basically this property of the Bessel function makes them that there are infinite number of roots are possible of this equation, J n x is equal to 0. For this equation, there are infinite number of roots are possible and all of these roots are corresponding they correspond to the eigen values of the problem.

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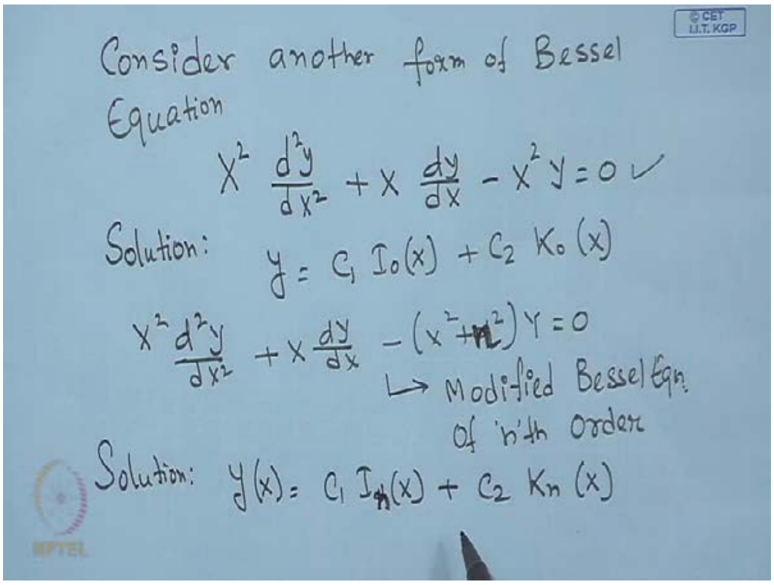

So, we will come to that later on, but let us look into the properties of J n and now let us consider the another variation of Bessel function or Bessel equation, consider another form of Bessel equation, the equation becomes X square d square y dx square plus X dy dx minus X square y is equal to 0.

So, if this is the form of equation, then the solution is in this form y is equal to c 1 I 0 x plus c 2 K 0 x. Now, for a general form, X square d square y dx square plus X dy dx minus X square plus alpha square times Y is equal to 0. Let us say x square plus n square to make it more uniform, now this equation is known as the modified Bessel equation, this is of zero th order, this is modified Bessel equation of nth order.

So, therefore, we will be getting the solution for this particular problem as y function of x is nothing but, c 1 i alpha x I n x plus c 2 K n x. So, the idea, the difference between the Bessel equation and modified Bessel equation is that, there will be minus sign and it will be plus. And in case of Bessel equation, the solution is constituted by J 0 J n and Y n functions, in case of modified Bessel equation the solution is composed of I n and K n functions, both appear in the solution if you work in the cylindrical polar coordinate system.

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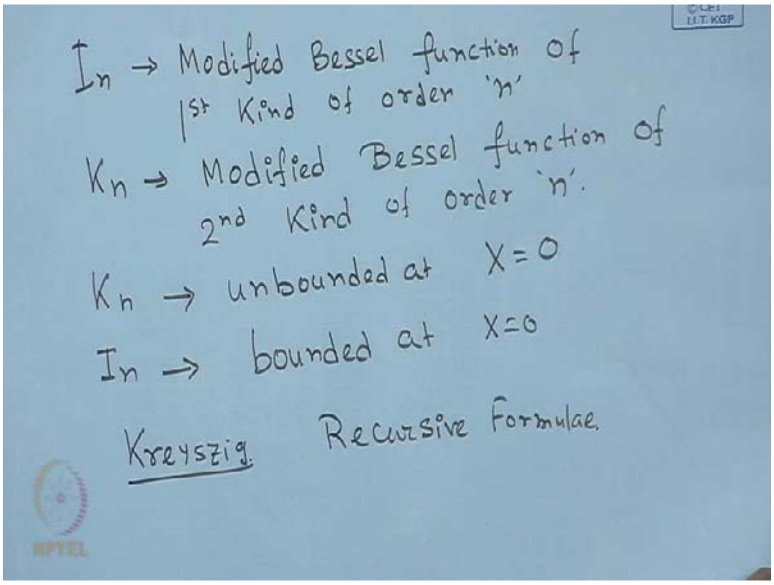

Now, I n is known as the modified Bessel function of first kind of order n and K n is modified Bessel function of second kind of order n K n. The important property is K n is unbounded at X is equal to 0 and I n they are bounded at X is equal to 0. Now, there are recursive formulas are available for J n and I n and these equations the various relations of Bessel functions modified Bessel functions are available in any standard text book of mathematical functions.

We can look into the book of Kreyszig and look into the properties of Bessel functions and modified Bessel functions of different orders, their recursive formulas are available to connect them up. The differentials of Bessel function, the differential of modified Bessel function all are available in any standard text book of mathematics of first year level.

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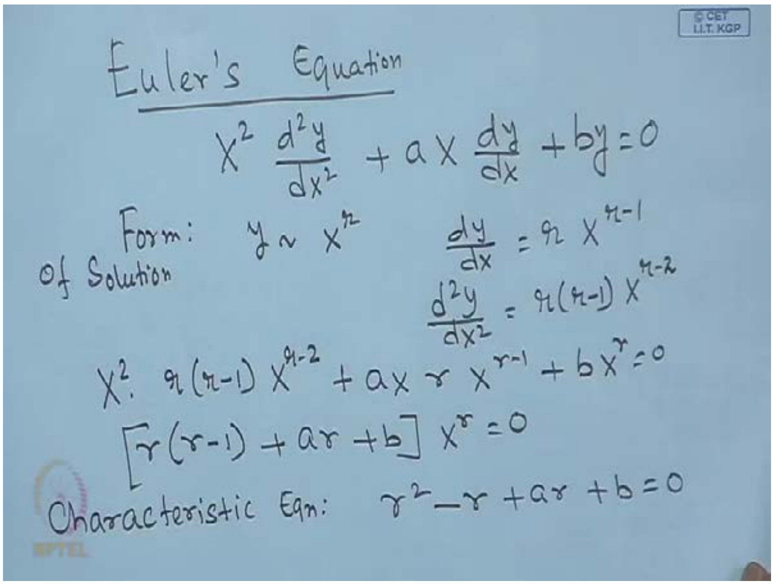

Next special ordinary differential equation that will be talking about is Euler's equation, the Euler's equations are in the form of X square d square y dx square plus a X dy dx plus by is equal to 0. Now, the form of the solution is the form as y is equal to X to the power r, this is the form of solution. If we put it that, then what is dy dx? dy dx is nothing but r X to the power r minus 1, one more differentiation, so d square y dx square is nothing but, r into r minus 1 x to the power r minus 2.

So, if we put it here in the governing equation, X square r r minus 1 X to the power r minus 2 plus a X dy dx is r x to the power r minus 1 plus b y is X to the power r is equal to 0. So what will be getting is that, you can in everywhere the X containing term appears to be X to the power r, so this becomes r into r minus 1 plus a r plus b multiplied by X to the power r is equal to 0. So, the characteristic equation we get is, r square minus r plus a r plus b is equal to 0. It is a quadratic in r, so therefore, there are 2 roots are existing, each root will be corresponding to each solution.

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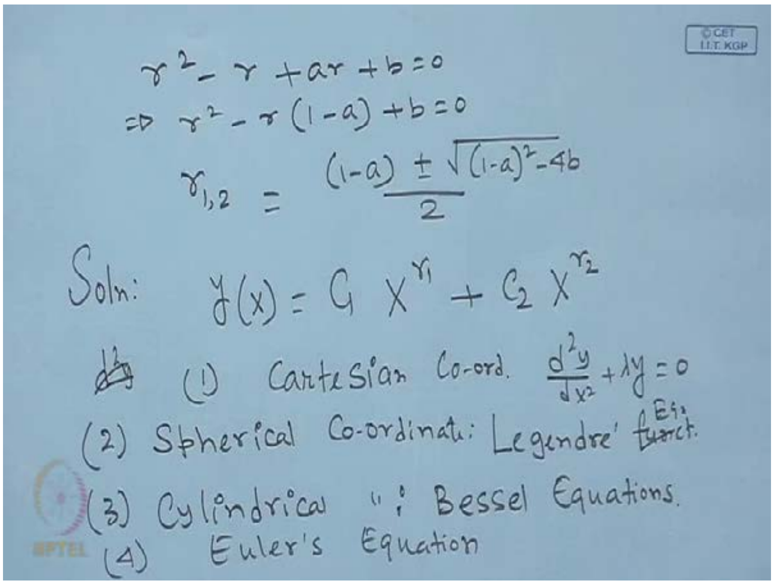

So, if you solve this equation, we will be getting r square minus r plus a r plus b is equal to 0. So you will be getting r square minus r into 1 minus a plus b is equal to 0; so you will be getting this is a quadratic 2 solutions, r 1 2 is equal to minus b plus minus under root b square minus 4 b divided by 2.

So, one root corresponds to plus, another root corresponds to minus, so, therefore, the solution of Euler's equation is that, y function of x c 1 X to the power r 1 plus c 2 X to the power r 2, where r 1 2 is given by the in terms of the known parameters a b etcetera.

So, these are three form of special functions, these are the four forms of special ordinary differential equations, we have talked about first one, we talked about d square y dx square. So, these are basically the Cartesian coordinate, d square y dx square plus lambda y is equal to 0. So, we have discussed different boundary conditions and the form of the eigen values and eigen functions in detail, then we talked about the deferential equation in spherical coordinate, this is given by the Legendre functions.

Next, we talked about the cylindrical coordinate. So, these are the Legendre equation and the solution is composed of Legendre function and the Legendre polynomial and third one we talked about, the cylindrical coordinate system. The governing equation that you will be getting the Bessel equations, these are the ordinary Bessel equations and modified Bessel equations and the solution will be composed of Bessel functions and modified Bessel functions of first kind and second kind.

And the fourth one, we just looked into the Euler's equation as we will be seeing later on in this course that, Euler's equation will be useful, whenever we will be talking about a spherical coordinate system, it will constitute a part of the particular solution. So, these are the special ordinary differential equations, the chemical engineering students and chemical engineers, they quite often come across in various chemical engineering processes.

So, these are the… whenever we are talking about the flow through a channel, we are talking about the rectangular coordinate or Cartesian coordinate, whenever we are talking about the discussing about the flow through a pipe or some kind of flow through a tube, then we will be talking about the cylindrical polar coordinate system, where the governing equations will be govern will be given by the Bessel equations. Whenever we will be talking about a spherical coordinate system for example, you would like to store a gas in a spherical container and you would like to find out the heat transfer characteristic, mass transfer characteristic or a spherical ball, you would like to find out the heat transfer characteristic.

So, they will be quite often, they will be utilized in the different applications like metallurgical applications, then we will be talking about the spherical polar coordinate system and the Legendre functions or Legendre equations becomes very important and they will play a big role in solving those equations. And Euler's equations also play a role, whenever we will be discussing the problem in a spherical polar coordinate system.

So, these geometrics, these coordinate system and geometries are quite common in chemical engineering applications and we have already seen, what the different governing equations will appear to characterize such systems.

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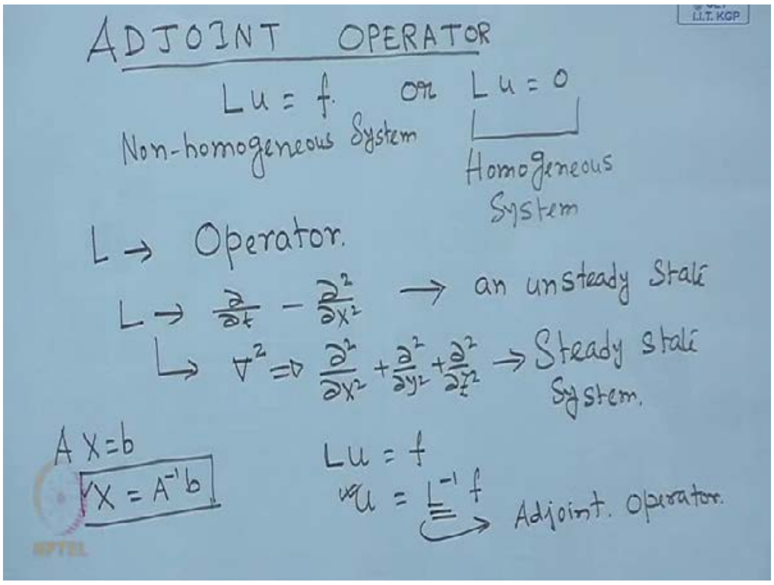

Next, we will just talk about the adjoint operator that is quite important whenever we are solving a chemical engineering system in continuous domain. So, we start with adjoint operator. Now, if in any chemical engineering system can be expressed in a mathematical form, in this form L u is equal to f or L u is equal to 0, this is for a generalized non-homogeneous system and this is for a homogeneous system, now where L is the operator.

Now, this operator will be the differential operator, it may be dels del del t minus del square del x square, so this is a typical operator to characterize an unsteady state system. L can be only a gradient operator del square, so it will be del square del x square plus del square del y square plus del square del z square in a three-dimensional process. So, this is typically an operator for a steady state system.

Now, if you look into the matrix operation, I will just bring a corollary of matrix operation A X is equal to b in a discrete domain, this is the matrix, what is the solution to this system? X is the solution vector, A is the matrix, b is the non-homogeneous vector or coefficient vector, so the solution is given as X is equal to A inverse b. So, we have to find out A inverse matrix inverse in order to guess the solution vector; similarly, in case of the chemical in continuous domain, L u is equal to f, so u is the solution, L is the operator, f is the non-homogeneous term.

So, what is the solution? The solution is obtained by L inverse f, now this L inverse in most of the cases are can be identically used for adjoint. So, in order to get this adjoint operator, if L is the operator, we find out L inverse as adjoint operator, so in order to find out a solution u, you have to determine the adjoint operator, so that you will be getting the complete solution. So, evaluation of adjoint operator is very important and in the continuous domain and once you will be evaluating the adjoint operator, you will be in a position to get the complete solution of the chemical engineering system.

So, I will stop the class at this point and in the next class, I will just take up and derive the general formulation of how to get an adjoint operator, given an operator for different boundary conditions as well. Then, we will look into the various theorems of eigen values and eigen functions, which will be quite important for the development of our system and the processes and solution of various chemical engineering equations. Thank you very much.