Advanced Mathematical Techniques in Chemical Engineering

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Lecture No. # 16

More Examples

Good morning everyone. So, in the last class, we have developed the theory of a stability analysis using the bifurcation theory or linear stability analysis. And we have seen how to characterize, how to model a chemical engineering system by ordinary differential equation and once we get that by solving those set of equations, you will be getting the steady states.

Now, the stability of these individual steady states is a very you know, it is a big problem in chemical engineering system; one has to run a particular system or a process under a particular steady state and that steady state has to be a stable steady state, until we do that, we cannot ensure the quality of the product that you are guide that we are getting out of the whole process.

Now, what have we done? We have developed the bifurcation theory and also we have looked into the parameters variation of the system parameters and how those system parameters will lead to stable steady state to unstable steady state, and these points are known as the bifurcation points, where the steady state becomes a stable steady state becomes an unstable steady state, because the parameters are changing their values.

Now, we have identified two bifurcations point - one is the saddle node bifurcation point and another is the half bifurcation points. In case of saddle node bifurcation points, the eigenvalues have to be real and in case of half bifurcation point, the eigenvalues will be complex conjugate. Now, if we summarize, what are the various steps involving into these processes? One first one will be, we will be getting the mathematical expressions to designate the particular system and we solve the steady state part of that of those equations in order to get the steady state.

In most of the chemical engineering processes, these equations will be leading to a set of ordinary - a set of algebraic equations may be non-linear, then one has to invoke Newton Raphson Technique or some numerical iterative technique to solve this set of algebraic equations. So, solutions of these equations will be corresponding to the steady state of the system. Now, what do we do? We take up each and individual steady state and evaluate, and check their stability.

So, the procedure for that is step number 2; the step number 2 will be doing will be first evaluating the Jacobian matrix, and the Jacobian matrix has to be evaluated at the steady state - at the constant steady state, and then we will be looking into the eigenvalues of this particular Jacobian matrix. And by looking into the sine of the eigenvalues, one has to identify whether that steady state is stable or unstable.

If eigenvalues are negative, they will be having a negative real part, then we will be getting a stable steady state. If the eigenvalues are complex conjugate with a negative real part, then the eigen, then the system becomes, then the concerned steady state is a stable steady state. If one of the eigenvalues is positive and all eigenvalues are negative, then again the system becomes unstable steady state.

Now, one can also look into the you know, change in parameters in the phase plane plot, and can identify the bifurcation points at which the state - the stable steady state. When these parameters will cross over the axis - imaginary axis, they will move the steady state moves over the right up plane and the real part becomes positive.

So, this transition occurs at the bifurcation points and there will be set of a particular relationships that exist among all parameters, where one can land up with the bifurcation point. So that is very important and we have to avoid that; so, therefore, we can identify what are the bifurcation points, we can test the various steady state and they are stability; we can always examine.

Now, if it is a two dimensional problem, then the problem becomes absolutely simple and you one will be getting the by looking into the trace value and determinant value of the Jacobian matrix, one can evaluate the stability of the steady state for this particular case; for a two dimensional problem, the trace has to be negative and determinant has to be positive, then we will be getting a stable steady state.

Now, for a multi-dimensional problem, one has to use the Rout Hurwitz criteria to determine the conditions, to evaluate the conditions of stability of the steady state we are concerning. So, in the last class, we have developed the full theory of linear stability analysis or the bifurcation theory, and then we took up some of the examples. And several examples we have taken up, and in the last example what we are solving? It was half done; we will be completing that problem. Look into one more problem and then move over to the partial differential equations in continuous domain.

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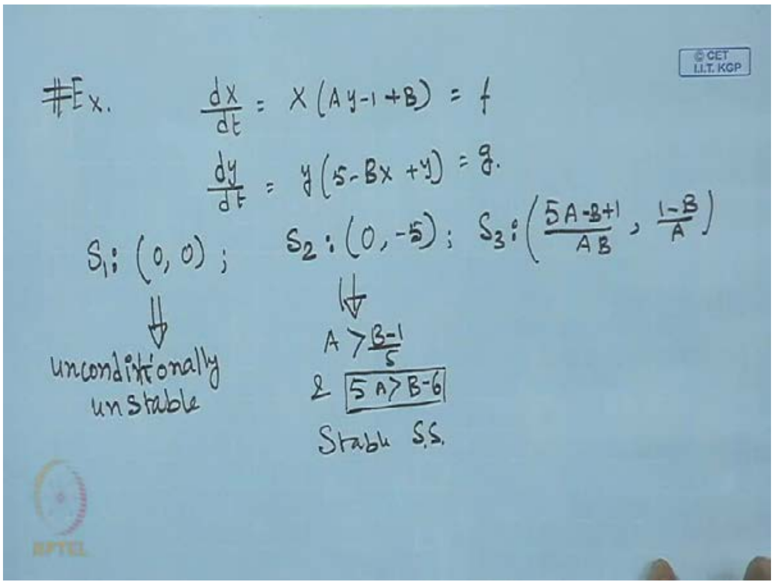

So, if you remember the example problem, we were looking into is that the system is designated by this two ordinary differential equations dx dt is equal to X A y minus 1 plus B that is equal to f, and dy dt is y into 5 minus Bx plus y that will be equal to g.

Now, there will be there are we have already solved this problem in the last class. There are three steady states available in this problem; the first steady state is S 1 is 0 0, the steady state number 2 - S 2 0 minus 5, and steady state 3 - S 3 is given by 5 A minus B plus 1 divided by A B and 1 minus B over A. So, we have already checked the stability of the first two steady state; the first steady state 0 0 was unconditionally unstable; we have evaluated that unstable, and this will be stable, if the following conditions will hold good.

If A is greater than B minus 1divided by 5, and 5 A is greater than B minus 6, then this is the condition, these two are identical conditions; so this will be most stringent condition.

So, subject to this, one has to get a stable steady state. Now, in today's class what we will be doing? We will be examining the steady state number 3.

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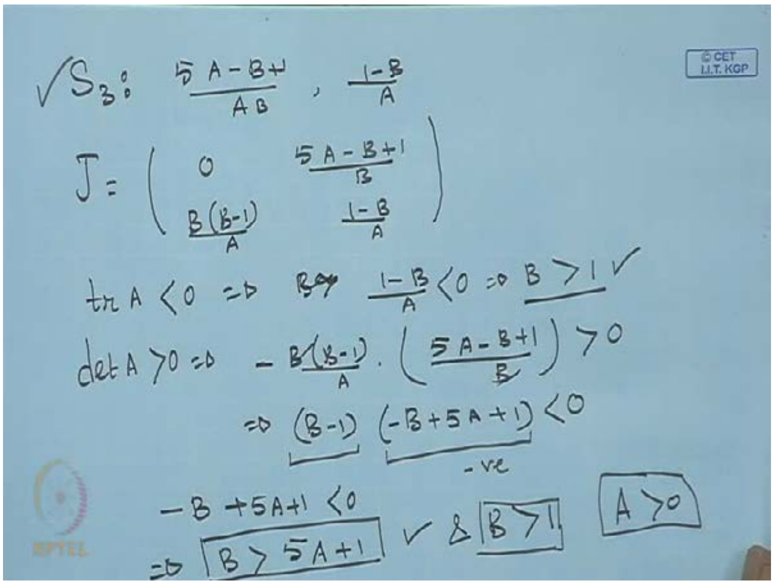

So, let us start with that, the steady state S 3 is given by 5 A minus B plus 1 divided by A B, and 1 minus B divided by A, this is the steady state x value, this is the steady state y value. So, we evaluate the Jacobian matrix at this particular steady state values. So, this becomes 0 5 A minus B plus 1 divided by B, and this will be B into B minus 1 divided by A, and 1 minus B divided by A.

So, now if you look into the trace of A that has to be less than 0; so, therefore, B is greater than so if trace is less than 1, less than 0 that means the two diagonal elements have to be added up. So, it will be 1 minus B divided by A should be less than 0; therefore, B is greater than 1. And the other condition is determinant of A is greater than 0; so, therefore, minus this into this is 0; so minus of this, so minus B into B minus 1 divided by A into 5 A minus B plus 1 divided by B that has to be greater than 0. So, this B will be cancelling out, A will be going to zero; so it will be B minus 1 then B minus 5 A or we can put it like this B minus 5 A minus B plus 1 should be…, so there is a minus sign; so this should be less than 0. So, this condition can be satisfied, but we have already seen that for a stable steady state, trace must be equal to 0 that means B must be greater than 1 that means in order to…; so this is always positive. Now, to get a negative number, it has to be negative then only the product will be negative.

So, therefore, in order to get the stability, we have we must have minus B plus 5 A plus 1 should be less than 0; so b should be greater than 5 A plus 1. So, if these two conditions are satisfied, simultaneously, B is greater than 1 and B is greater than 5 A plus 1, and A is always if you remember, A is always positive and it is a non-zero positive parameter; so, therefore, B is greater than 5 A plus 1, will be always satisfied.

So, using these two conditions B has to be positive and it has to be greater than 1, and secondly it has to be greater than 5 A plus 1. So, if these two conditions are satisfied, then with the steady state, S 3 is stable and we will be getting a very stable steady state.

Now, we will be looking into the next problem; so that completes this problem the then we will go to the next problem.

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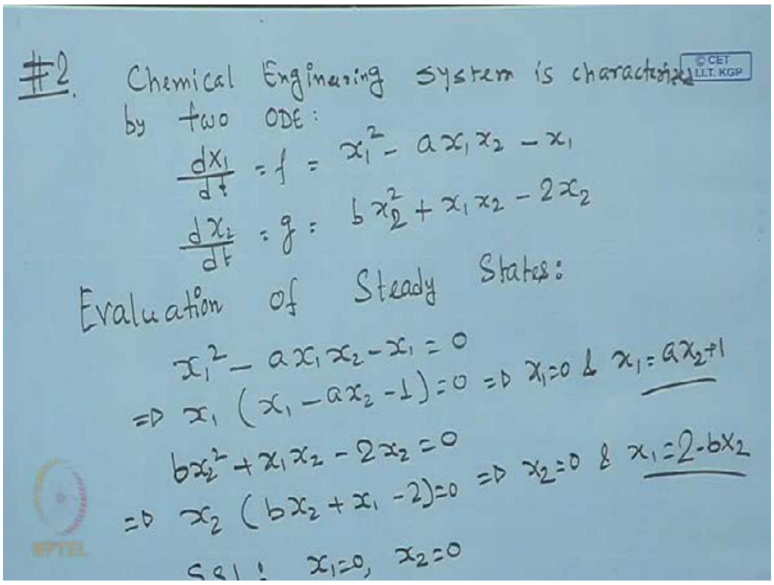

Next problem is, we the chemical engineering system is characterized by two ordinary differential equations; these are dx 1 dt is equal to f is equal to x 1 square minus ax 1 x 2 minus x 1, and dx 2 dt is equal to g is equal to b x 2 square plus x 1 x 2 minus 2 x 2. So, we can and these A B are the parameters and these parameters are positive parameters in the system. So, one can get the you know various steady states and check into the solution of the steady state. Now, first step will be evaluation of steady state; so, we put dx 1 dt equal to 0 and dx 2 dt equal to 0. So, what we will be getting from the first equation is x 1 square minus ax 1 x 2 minus x 1 should be equal to 0; so take x 1 common, so it will be x 1 minus ax 2 minus 1 is equal to 0; so that is equation number 1.

So, we will be getting either x 1 equal to 0 or x 1 is equal to ax 2 plus 1. Now, from the equation number two, we will be getting bx 2 square plus x 1 x 2 minus 2 x 2 is equal to 0; so, therefore, you can take x 2 as common, bx 2 plus x 1 minus 2 is equal to 0. So, therefore, from this we will be getting x 2 equal to 0 and x 1 is equal to 2 minus bx 2; so, we will be getting two steady state - one is x 1 is equal to 0 and another is x 2 is equal to 0.

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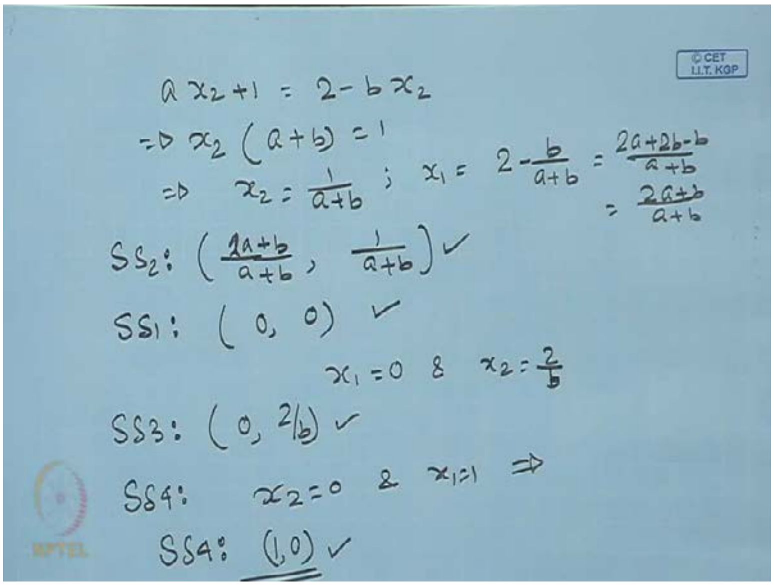

So, we can identify the steady state 1 as, x 1 is equal to 0 x 2 is equal to 0. Now, one can solve these two equations simultaneously and can get the second steady state; if we really solve them, it will become ax 2 plus 1 is equal to 2 minus bx 2; so, we can take x 2 common change over the sides this becomes a plus b and it will be 2 minus 1 is 1

So, x 2 will be 1 over a plus b and what is x 1? x 1 if you remember, this becomes 2 minus bx 2; so, b divided by a plus b, so it becomes 2 a plus 2 b minus b divided by a plus b; so this will be 2 a plus b divided by a plus b. So that will be second steady state.

So, steady state 2, will be first steady so this will be 1 over x is equal to 2 a plus b, so it will be 2 a plus b divided by a plus b, and x 2 is 1 over a plus b; so this is steady state number 2. The first steady state, we have already seen 0 0 is the first steady state, then if you check that x 1 is equal to 0, and x 2 is equal to 2 by b is another steady state, because if you look into this equation x 2 is equal x 1 is equal to 2 minus x 1 is equal to 2 minus bx 2. So, putting x 1 equal to 0, you will be getting another solution 2 by b. So, steady state number 3 will be 0 and 2 by b; so this will be the third steady state.

Similarly, you can get another steady state that is steady state number 4; steady state number 4 will be x 2 equal to 0. So, if x 2 equal to 0, if you look into the expression of f, if x 2 is equal to 0 and you will be getting g; g will be satisfied and if x 2 is equal to 0 then you will be getting x 0 is equal to 1.

So, if you look into the equations dx 1 dt is equal to 0 and dx 2 dt is equal to 0, you will be seeing that X 2 is equal to 0 and x 1 is equal to 1 will give another steady state; they will satisfy both steady state equation. So, S S 4 the steady state number 4 is given by 1 0.

So, we can identify that there are four steady states into this particular problem, then we will take up each and individual steady state and check their stability. So, next, we will do; so we have identified the steady state; next, what we will do? We will be evaluating the Jacobian matrix, and evaluate each and every for each and every steady state, we will evaluate the Jacobian matrix.

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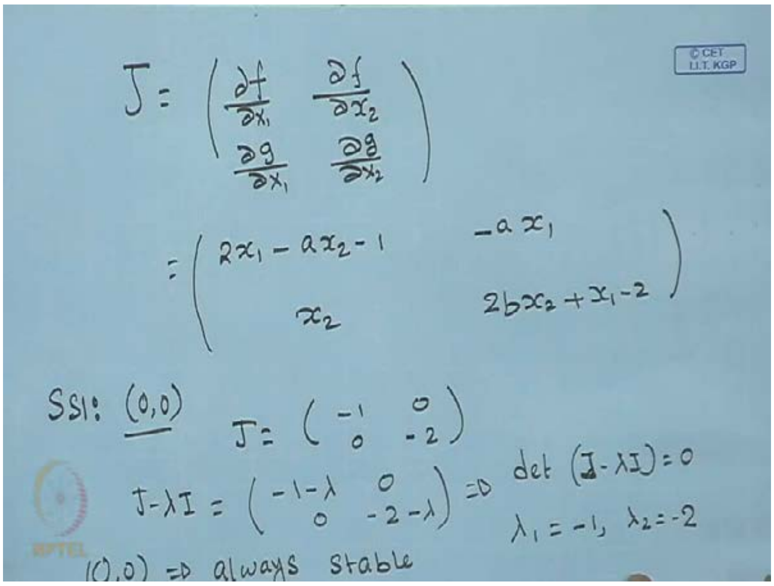

Next, we evaluate the Jacobian matrix that will be nothing but partial derivative of f with respect to x 1 del f partial derivative of f with respect to x 2, partial derivative of g with respect to x 1 partial derivative of g with respect to x 2; so that is the Jacobian matrix.

If we evaluate all these partial derivatives and put them into here, in the elements of the matrix this becomes 2 x 1 minus ax 2 minus 1 minus ax 1, x 2 2 bx 2 plus x 1 minus 2. So, this is the Jacobian matrix. Now, we take up individual steady state and check their stability. First steady state, we talk about is 0 0; so j becomes minus 1 0, 0 and minus 2. We evaluate the J minus lambda I, the eigenvalues, so it becomes minus 1 minus lambda 0, 0 minus 2 minus lambda; so we evaluate the eigenvalues. Put the determinant of J minus lambda I is equal to 0; so, therefore, we will be getting lambda 1 is equal to minus 1 and lambda 2 is equal to minus 2.

So, this steady state is unconditionally stable. 0 0 is always stable, you can interpret this from the determinant value and trace value, trace did not turns out to be negative, which has to be the case and determinant turns out to be positive; therefore, this steady state S S 1 is unconditionally stable.

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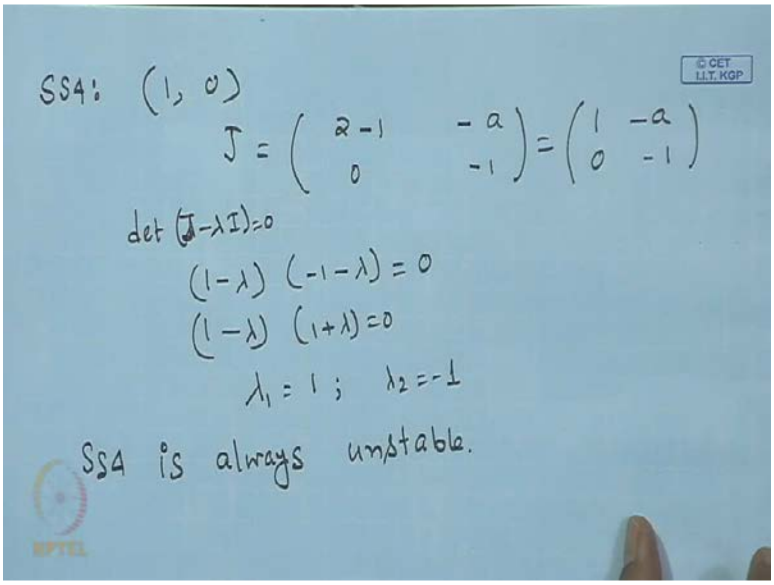

Next, we check the second steady state. So, we take up steady state number 4, because it has only value 1 and 0 that is the steady state value. So, evaluate the Jacobian matrix, the Jacobian matrix becomes 2 minus 1 minus a, 0 and minus 1. So, this becomes 1 minus a, 0 and minus 1. So, if you look into determinant of J minus lambda I is equal to 0, if you put that, then what will be getting is that 1 minus lambda minus 1 minus lambda minus 0 into this, so this should be equal to 0. So, 1 minus lambda and 1 plus lambda is equal to 0.

So, you will be having two roots of this equation; so lambda 1 will be 1 and lambda 2 will be minus 1; since, one of the root is positive, then 1 4, steady state 4 is always unstable and unconditionally unstable, we can say it.

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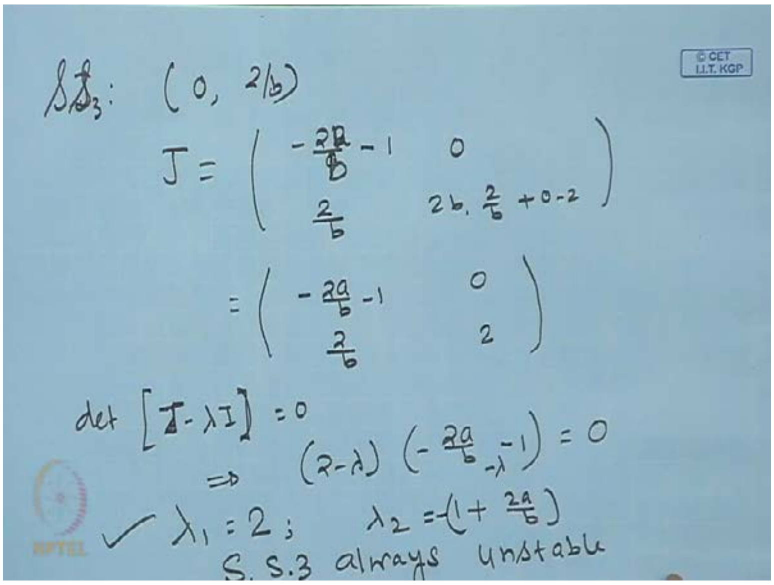

Next, we check the third steady state; the next steady state will be 0 and steady state number 3. So, it will be 0 and 2 by b and this will be given by the… Now, we evaluate the Jacobian matrix at these values; so it will be minus 2 b by a minus 2 a by b minus 1 2 2 by b, then 2 b into 2 by b plus 0 minus 2. So, this becomes minus 2 a by b minus 1 0 2 by b and 2; so 4 minus 2 it will be plus 2.

So, we will be getting the determinant of J minus lambda I should be equal to 0. So, if you do that what will be getting is that 2 minus lambda into minus 2 a by b minus 1 minus lambda is equal to 0. So, lambda 1 will be 2, and lambda 2 will be 1; so lambda 2 it will be 2 a minus b minus 1 minus lambda; so lambda 2 will be 1 minus will be common 1 plus 2 a by b.

But since, you will be having one eigenvalue, so there will be minus sign here, so this will be positive; so it will be lambda 2 will be negative, but lambda 1 is positive. So, therefore, steady state 3 will be unconditionally unstable, is steady state 3 is always unstable. So, likewise, we can evaluate the steady state 4 as well, the steady state 4 becomes the complicated one.

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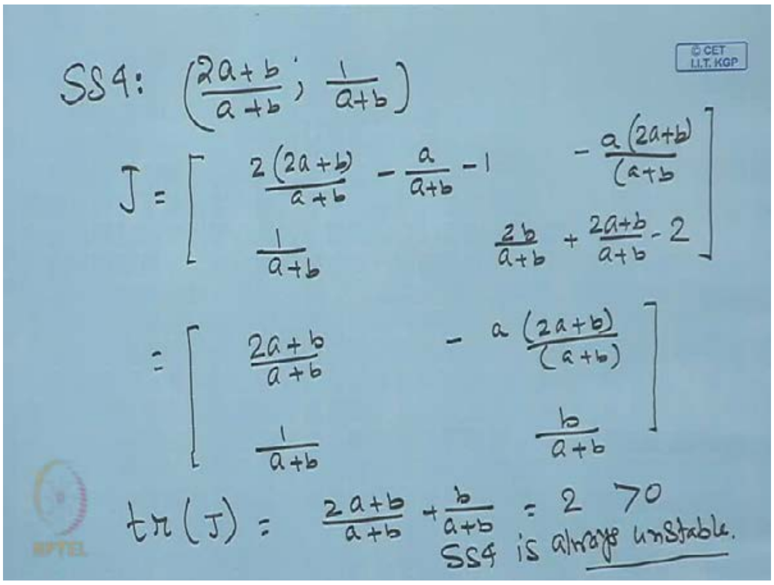

So, S S 4 is 2 a plus b divided by a plus b and 1 over a plus b. So, therefore, we evaluate the Jacobian matrix at this; so this becomes 2 into 2 a plus b divided by a plus b, minus a divided by a plus b minus 1 minus, a into 2 a plus b divided by a plus b, 1 over a plus b, then this becomes 2 b by a plus b plus 2 a plus b divided by a plus b minus 2. We simplify all these and I am just writing the final expression of Jacobian matrix; this becomes 2 a plus b divided by a plus b and 1 over a plus b it is 1, minus a into 2 a plus b divided by a plus b and this will be b divided by a plus b.

So, if you look into the do not worry about anything else if you look into the trace of this Jacobian matrix this becomes 2 a plus b divided by a plus b plus b into a plus divided by a plus b; so it becomes 2; so trace is 2 which is greater than 0. So, steady state 4 is always unstable.

So, therefore, this way we can evaluate the so this that complete this problem and this problem demonstrates, how the various steady states of a particular problem can be evaluated - can be checked for its stability. And also, we can look into the combination of the parameters for which the system becomes stable or the steady state becomes stable or unstable.

So, we finish the stability analysis by bifurcation theory or linear stability analysis for any chemical engineering system for a 3 into 3 matrix or 3 into 3 variables or multi-dimensional problem. One can take recourse to the Routh Hurwitz criteria or Routh

Hurwitz table to evaluate the conditions on the steady states, the stability of the steady state.

Next, we move towards, move forward and we will move towards the differential equations, and first we will talk about some of the basic definitions of the differential equations and we will be mostly talking about partial differential equations. And it is understood that most of you have already done a lots of you know, solutions for the ordinary differential equations in your undergraduate study and we will be looking into the solution of the partial differential equations.

First we will characterize the partial differential equations; we will be looking into various properties of partial differential equations, we will characterize them and then we will be looking into solution techniques. We will be not only equations we will be talking about the boundary conditions; we will classify the boundary conditions and see how these boundary conditions will be appearing for different physical situations under chemical engineering applications.

And then we will be looking into the solutions; we will be taking recourse to some of the techniques. One is the separation of variable techniques, then similarity solution, then we will be looking into laplace transform, we will be looking into the fouriers transform, then we will see the general method of solution for non-homogeneous partial differential equation using greens function.

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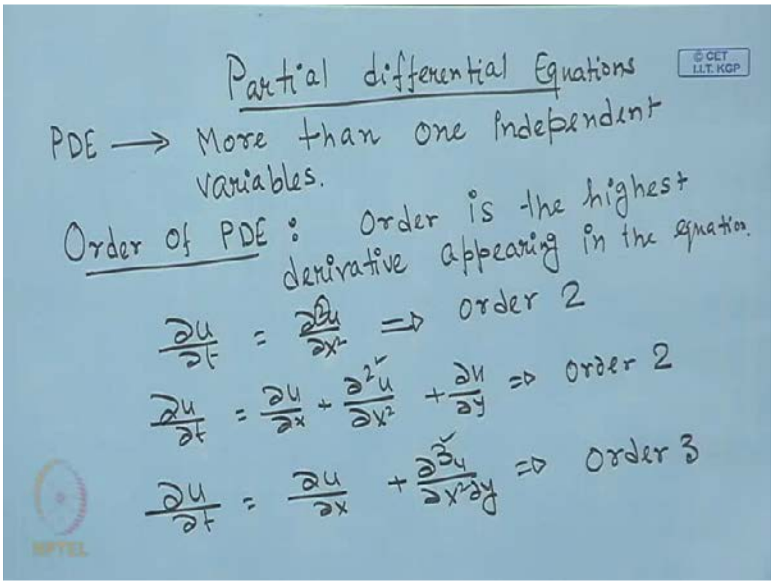

So, let us with that preamble, we will start the portion of partial differential equation. So, partial differential equations are basically equations, which will be having more than one independent variable; if your system or equations have more than one independent variable, then it is called a partial differential equation.

Next, we talk about the order of P D E - order is the highest derivative appearing in the equation appearing in the equation. For example, this equation del u del t is equal to del square u del x square; in this P D E, the highest derivative occurring is second order; so the order is 2. Next, del u del t is equal to del u del x plus del square u del x square plus del u del y; since, the highest derivative occurring is the second order; so, again this is having order 2. For example, del u del t is equal to del u del x plus del cube u del x square del y, then the highest derivative that is appearing is 3; so it has an order of 3.

So, the highest derivative that is appearing in the partial differential equation is defined as it’s order, then we will discuss about the linearity and nonlinearity of the partial differential equations.

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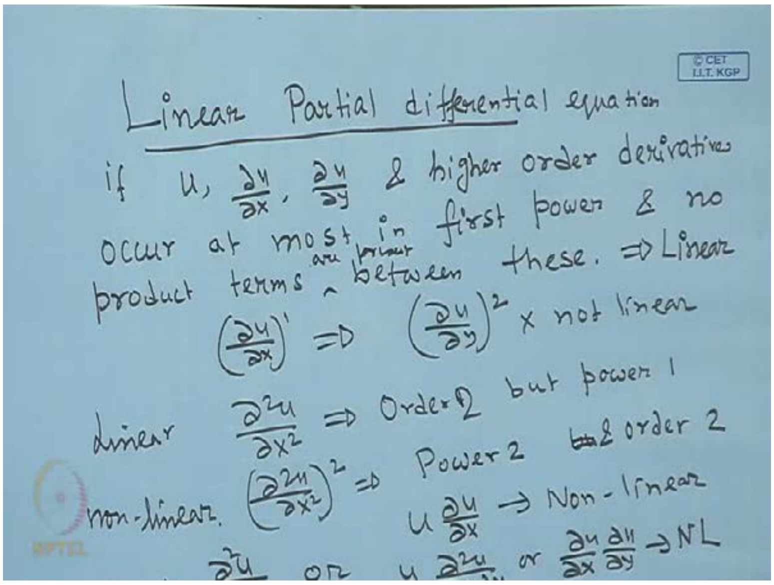

So, first we talk about the linear partial differential equation; we call that partial differential equation as linear, if u, del u del x, del u del y and higher order derivatives occur at most in first power and no product terms exist or present between these, then we call these partial differential equations as linear, that means power means del u del x raise to the power 1 if that is the case, then this is a linear partial differential equation.

Similarly, if we have a term, del u del y square, then it is not linear. Similarly, if we have a term, del square if we have a term del square u del x square this is having order 1, but power 1. (Refer Slide Time: 32:27) del square u del x square square, so this will be having this is order the del square u del x square is order 2, but power 1; in this case this will be order 2, but power 2; order is also 2. So, this is linear, this is non-linear.

If any product term is present like, u del u del x, then it is non-linear. If your product, if any product term is present like, del u del square u del x square or u del u del x square or u del square u del x del y or del u del x del u del y again, they are non-linear. So, whenever the product terms are absent, whenever the power is 1, then the partial differential equation is termed as linear partial differential equation.

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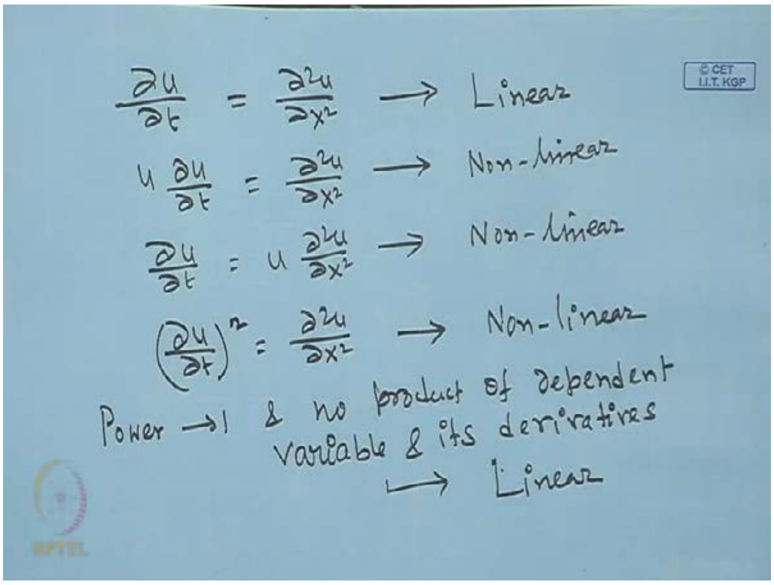

We will take away take up some of the examples, del u del t is equal to del square u del x square, it has order 2, but power 1 and there is no product term present; so this is a linear P D E. u del u del t is equal to del square u del x square again, here, the product term is present between the dependent variable and its derivative and the order 2; so, therefore, this is non-linear, because of the product term present. Third one is del u del t is equal to u del square u del x square again, this is order 2, but the product term is present u del square u del x square; so, therefore, again this is non-linear. del u del t square is equal to del square u del x square, so again, the power is 2 of this, although the order is 2, but this is again since, power is not 1; so it is non-linear.

So, the important thing is, the power should be 1 and not a product of dependent variable and its derivatives; if that is the case, we call that partial differential equation as linear partial differential equation.

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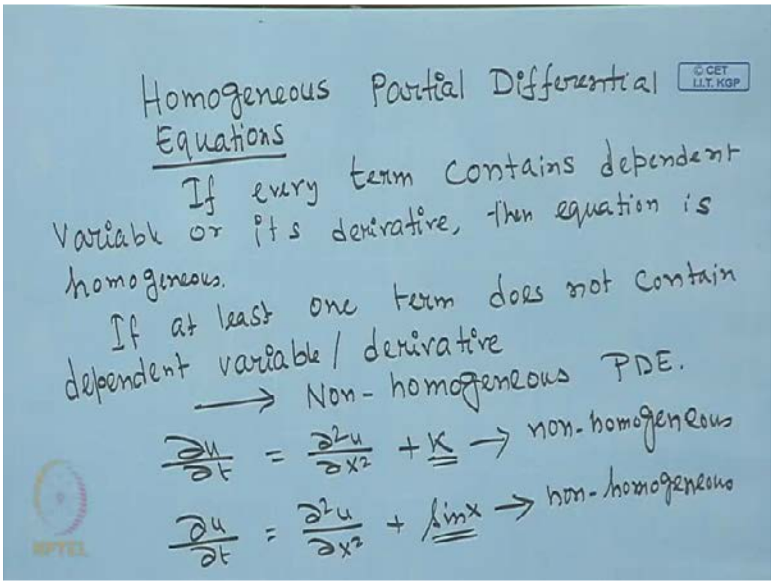

Next, we talk about the homogeneous partial differential equation. In case of homogeneous, if every term contains in dependent variable or its derivative, then it is called homogeneous, then the equation homogeneous, that means every term of the equation must be a dependent, must be containing depending variable or its derivative.

If at least, one term does not contain dependent variable or its derivative, then this is non-homogeneous PDE. So, I will take up some example, del u del t is equal to del square u del x square, some constant K. Now, in this equation, this term constant K does not contain the dependent variable u or it is derivative so the, because of this, equation becomes non-homogeneous. del u del t is equal to del square u del x square plus sin x now, this term contains the independent variable, but this term does not contain the dependent variable; so this is again a non-homogeneous equation.

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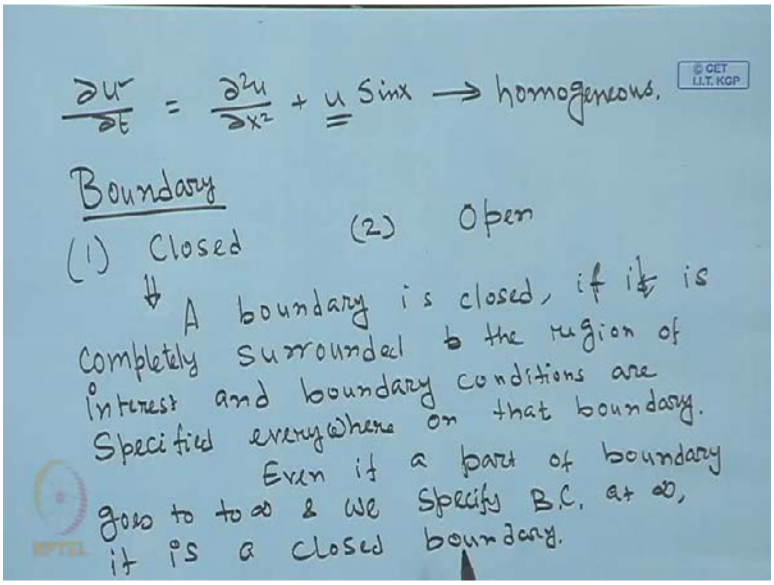

On the other hand, just look into this example, del u del t is equal to del square u del x square plus u sin x, in this equation all the term contains the dependent variable u and it is derivative contains u; so again, this is homogeneous.

So, these are the various types of general types of equations we are talking about, then we will look into the boundaries, equations - partial differential equations cannot be solved without the boundaries.

Now, there are two types of boundaries generally, we consider one is the closed boundary, another is the open boundary. For a closed boundaries, the closed boundaries are a boundary is term is closed boundary is closed, if it is completely surrounded the region of interest and boundary conditions are specified everywhere on that boundary.

So that particular boundary is called as the closed boundary, even if a part of boundary goes to infinity and we specify boundary condition at infinity, it is a closed boundary. If a boundary condition is specified at infinity, if that is specified, then it cannot be an open boundary, it will be a closed boundary in that case as well.

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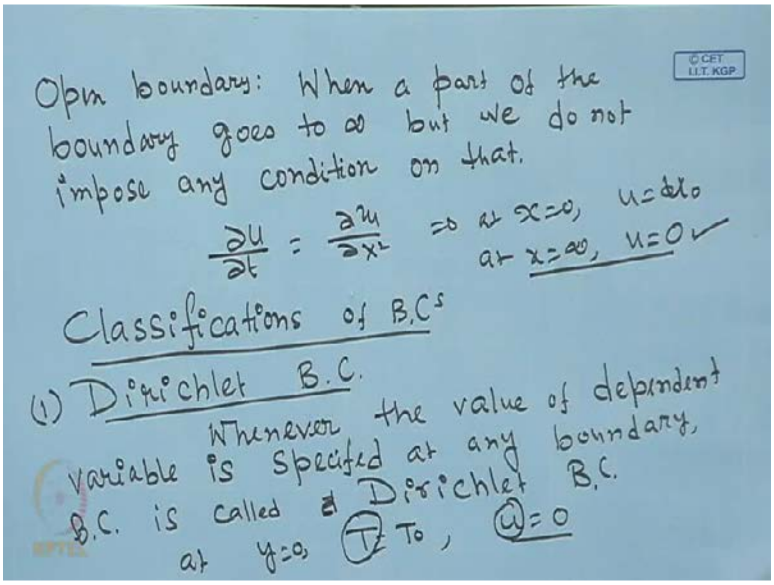

Next, we look into an open boundary. What is defined as an open boundary? The open boundary is defined as, when a part of the boundary goes to infinity, but we do not impose any condition on that, then the boundary is called the open boundary.

So, I will give an example for this particular problem. Let us say, del u del t is equal to del square u del x square. Now, in this case, at x is equal to 0, u is equal to 0; at x is equal to infinity let say, at x equal to 0, u is equal to u naught; at x is equal to infinity u is equal to 0. Now, although this is boundary is situated at infinity were since, this condition is specified; this is a case of closed boundary condition.

On the other hand, if you look into the other boundary of the t that is open and that goes to infinity, but we cannot impose any condition on that t. So, therefore, the other boundary condition on t at infinity is an open boundary condition.

Next, we look into the several types of boundary conditions - classifications of boundary conditions. First boundary condition is Dirichlet boundary condition. Now, in this case, whenever the value of dependent variable is specified at any boundary, then this boundary condition is called Dirichlet boundary condition. For example, at y is equal to 0, T is equal to T naught; this is an example of Dirichlet boundary condition.

At y is equal to 0, u is equal to 0, so this is an example of Dirichlet boundary condition where the value of the dependent variable is specified, whether it is 0 or some specified value; so, then we call this boundary condition is dirichlet boundary condition.

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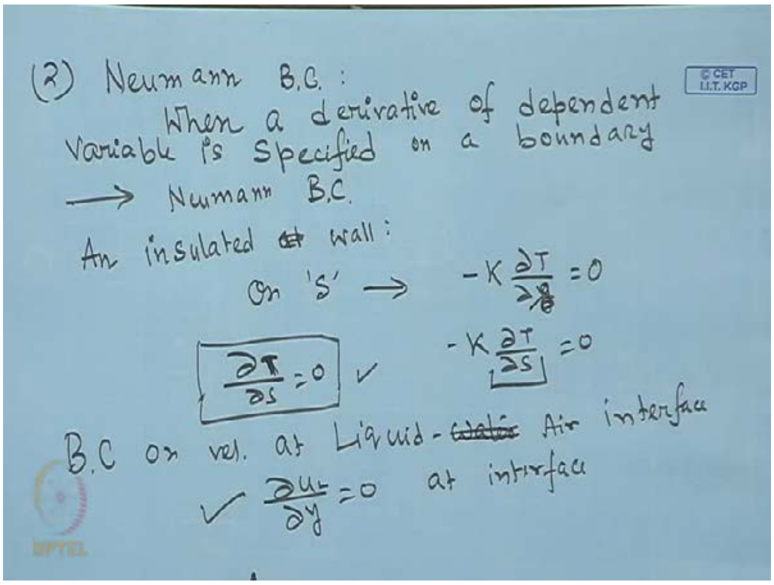

Next, we talk about next boundary condition is Neumann boundary condition. Neumann boundary condition is whenever a derivative of dependent variable is specified on a boundary we call that boundary as Neumann boundary condition. That means a physical example in chemical engineering system is, an insulated wall, an insulated wall means at a boundary on some surface S, you have minus K del T del y will be is equal on a surface s will be minus K del T del s is equal to 0, where s is the normal direction on that surface. So, therefore, the derivative is defined on… So, K is being constant or if it is not a constant does not matter, this becomes del T del S equal to 0. So, this is the derivative of the derivative of the dependent variable is specified on this boundary; so this is a Neumann boundary condition.

For example, another example is the boundary condition on velocity at liquid air interface let us say, air water interface in that case, we write del u in the liquid del y is equal to 0 at interface, this comes because of the matching of the shear stress at the at the interface, but the viscosity values So, this velocity gradient will be multiplied by the viscosity to get the shear stress, but the viscosity in the air is too order of magnitude less compare to that of water. So, we can approximate; we can neglect that part and we can approximate del u l in the liquid del y is equal to 0. So, again the derivative of the dependent variable is specified at this boundary; therefore, this boundary condition is a Neumann boundary condition.

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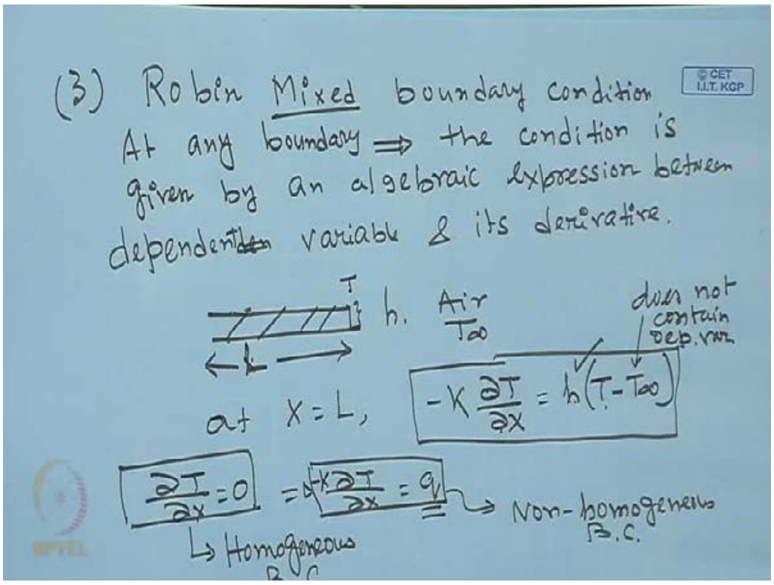

Next, one is Robin Mixed boundary condition. In this case, at any boundary, the condition is given by an algebraic expression between dependent variable and its derivative; whenever a dependent variable and its derivative both are connected by a simple algebraic equation and that is the condition that is specified at the boundary, then we call that boundary as a Robin Mixed boundary condition.

So, it is basically mixture of Neumann boundary condition and Dirichlet boundary condition. For example, we talk about a heat surface, a fin may be and that the age of the fin is exposed to air; air is having a temperature T infinity and at their particular point the at the particular boundary, let us say, at x is equal to L the temperature is T and h is the heat transfer coefficient, then that the steady state, whatever the heat that has been come that has come by conduction is taken away by the convection of the air.

So, minus K at the boundary, let us say, X is equal to L minus K del t del x that is the heat that has appeared at this boundary by conduction should be taken away by convection of air that is ambient air. So, h into T minus T infinity, h is the heat transfer coefficient; therefore this boundary condition is a mixture of dependent variable T and it is derivative del t del x and it is given by an algebraic equation; so, this is an example of robin mixed boundary condition.

Now, in this the case like del t del x is equal to 0 it is a Neumann boundary condition; this is a homogeneous boundary condition. Similarly, if you have del t del x is equal minus k del t del x is q, then because of this term, this becomes a non-homogeneous boundary condition.

So, this becomes a homogeneous boundary condition, and this becomes a non-homogeneous boundary condition that means even in the boundary condition, if there is any term present, which does not contain the dependent variable, then we call that equation as homogeneous boundary condition. For example, in this equation, there is one term there is at least there is no term that is present which contains the, which does not contain the dependent variable or it is derivative; so this is a homogeneous boundary condition.

On the other hand in this equation, there is at least one term is present, which does not contain the dependent variable and its derivative; so this is a non-homogeneous boundary condition. Now, in this equation there are three terms - two terms on the right hand side, one term on the left hand side; the first term on the left hand side, it contains a derivative of the term, on the left hand side contains a derivative of the dependent variable T.

The first term on the right hand side, it contains the dependent variable T, h times t, and the second term on the right hand side, it contains a constant term h into T infinity, which does not contain the dependent variable. So, this term does not contain dependent variable; therefore, this is a non-homogeneous term, and this boundary condition is a non-homogeneous boundary condition.

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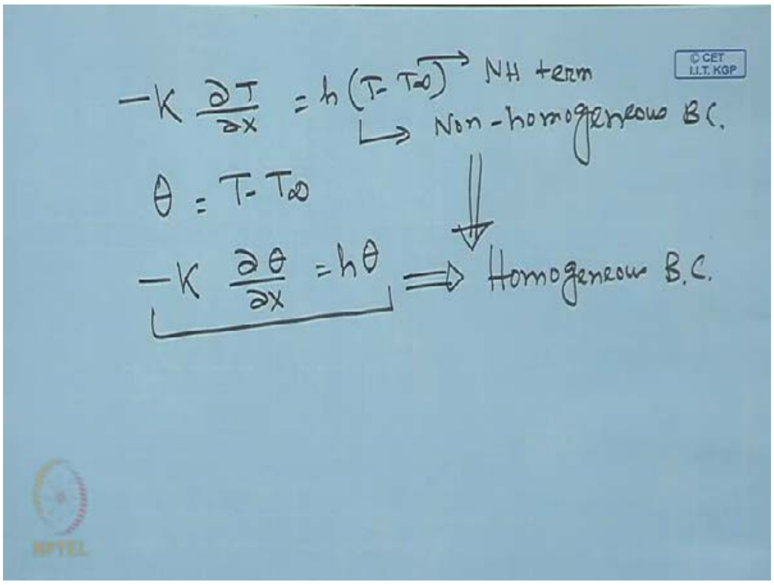

On the other hand, if we can make the non-homogeneous boundary condition, we can make it homogeneous minus K del T del X is equal to h T minus T infinity, so this is a non-homogeneous boundary condition; this is the non-homogeneous term. If we now, define a theta, such that theta equal to T minus T infinity, then this equation, this boundary condition becomes minus K del theta del x is equal to h into theta, but in this particular form of the equation, there is no term present, which is not a function of theta or it is derivative.

Now, all the terms, there are two terms present in this equation, both the term contains either the dependent variable theta or its derivative; therefore this equation becomes a homogeneous boundary condition. So, we can convert the non-homogeneous boundary condition into homogeneous boundary condition by defining an appropriate term.

So, I stop here at this point; we take up some more characteristics of the partial differential equations in the next class.

Thank you very much.