Advanced Chemical Reaction Engineering
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Lecture - 20
Energy Balance V: Stability Analysis of Exothermic Stirred Tank

In this lecture we will be looking at stability analysis of exothermic stirred tank. So, our system looks like this.

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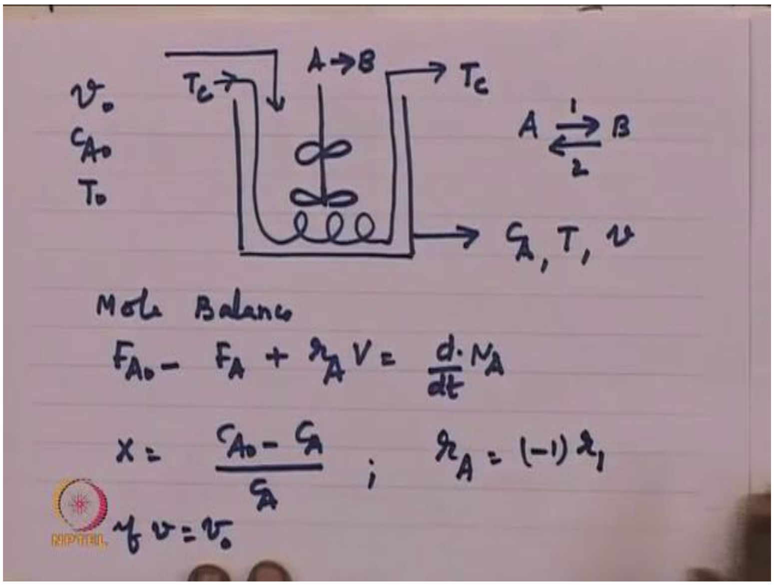

Let us look at a stirred tank scot; let see a cooling system, you have feed coming in products going out, feed is v naught C A naught and T naught it is temperature. We have C A naught becomes C A T, and let us say v is the object flow and T C temperature at which the cooling is coming. And, the flow of coolant is considered to be quiet large so, that the T C does not change all that much. So, as far as our analysis is concerned; we will assume it is reasonable the same that is the stirrer which keeps the flow it is fell mixed. So, that you have A C S T r.

So, we write the mole balance our reaction; let say A goes to B single independent reaction, or even if it is A in this form also there is only 1 independent reaction. So, we do the treatment for the case of 1 independent reaction say A goes to B. So, the system we consider is A going to B. So, we have mole balance which is input, output plus generation equal to accumulation. Let say A variable X define the C A 0 by C A divided by C A. This variable X has meaning of conversion at steady state; the during the unsteady state it should be treated as variable define by this relationship. So, suppose we say that volumetric flow is v equal to v naught means; what we are saying is, if v equal to v naught this equation can be written as v naught C A naught minus v naught C A minus of r 1 V. Because r A the rate of formation of A is given as minus of 1 times r 1, the rate, intensive rate of reaction A going to B, ok.

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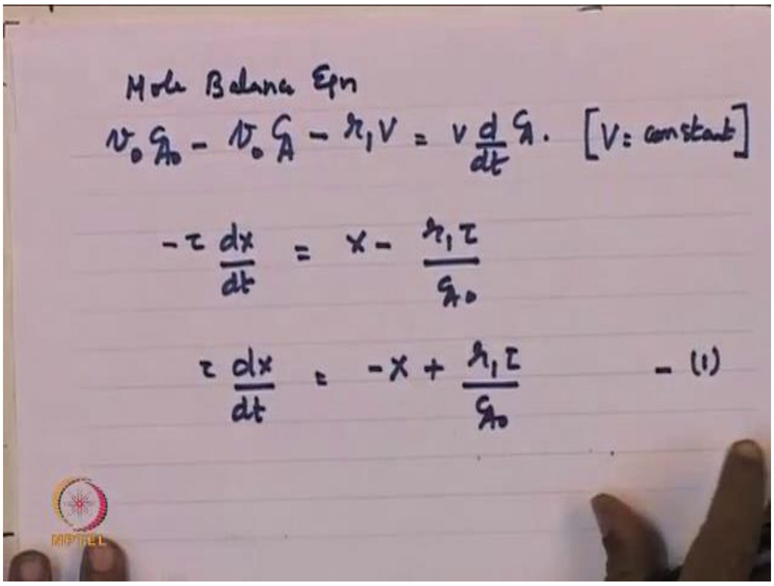

So, that this becomes equal to v times d by d t of C A. V is assume constant, what we saying is that; the equipment where we conduct the reaction that volume does not change during the reaction. So, we can simplify this and write it as minus of tau d X d T equal to X minus of r 1 tau divided by C A 0. Let us just check if this is correctly done, see if we divide throw out by v 0 this become tau that is fine. And, then C A naught minus of C A divided by C A naught becomes X. So, this X is correct, minus r 1 tau v and, C A equal to fine the relationship is fine. So, I will just put it in this form, d X d t is equal to minus of X r 1 tau by C A 0, this is our equation 1. Within balance so, this is the mole balance equation.

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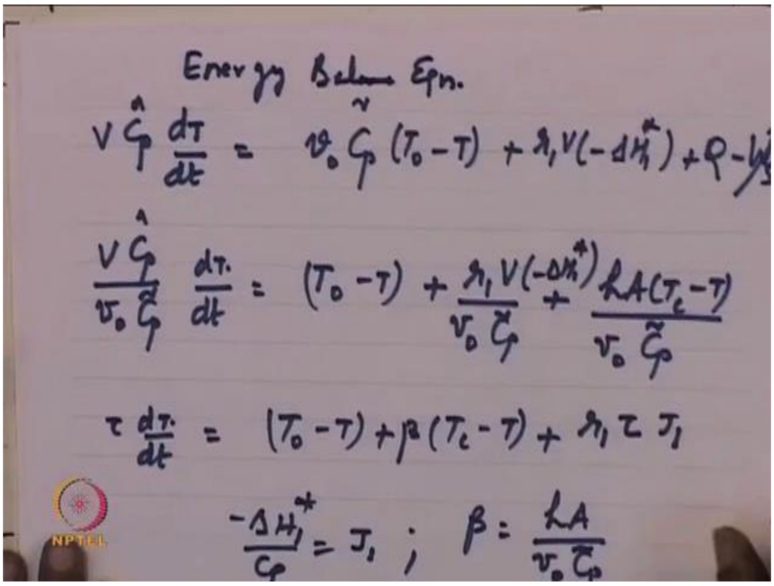

Our next equation is the energy balance equation, which we would write energy balance equation looks like this, we have written it before. So, let us V time C P volumetric specific heat d T d t so, the rate of change of temperature this is volumetric specific heat. v naught C P T naught minus of T plus minus of delta H 1 star plus Q minus V, we say this is not important ok. And then, if you divided throughout by v naught C p divide; we get V divided by C p divided by v naught C P d T d t, there is first term equal to T naught minus of T plus r 1 V divided by v naught C p plus Q. I will denote Q as H A times T C minus of T divided by v naught C p.

So, essentially dividing throughout by v naught C p so, the first term on the left hand side becomes d T d t equal to T naught minus of T and this term H A by v naught C p. Notice here H A by v naught C p is dimension less. We can easily check that so, I will put this as beta T C minus of T plus r 1 sorry, r 1 v minus delta I forgotten that term minus delta H 1 star here. So, you have r 1 tau and this I will call it as J 1 where, minus delta H 1 star by C p volumetric J 1, and beta equal to h A by v naught C P these are the 2. So, energy balance equation and this is energy balance equation. We can simply this further and put it in slightly more convenient form which we will do now.

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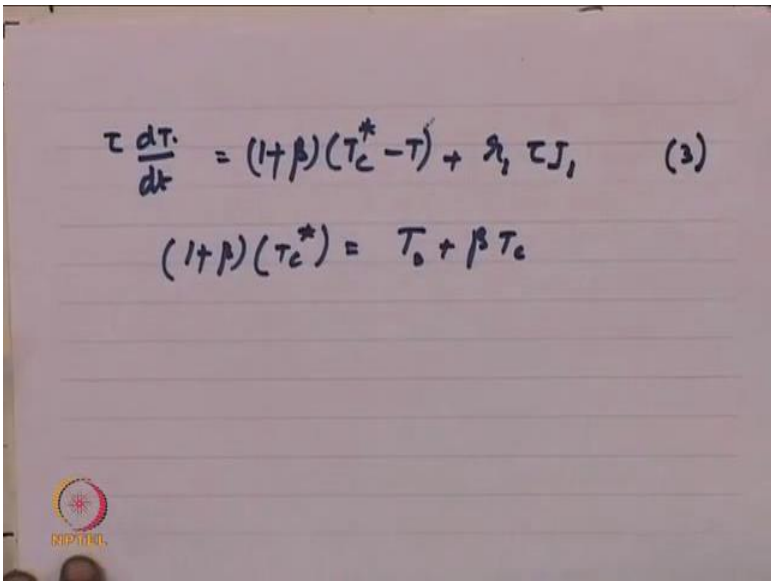

So, what we write this as tau d T d t that is first term; please notice here, our first term this is tau d T d t I am not change this. I want to combine this term with this second term. So, I am combining the first in the second term and writing it is 1 plus beta times T C star minus of T plus r 1 tau J 1 where, 1 plus beta times T C star equal to T naught plus beta T C. We have done please notice here, what we have done is can we see here we cannot see we cannot see very well you cannot see very well. What I am saying here is A following. So, I am combining these 2 terms and writing it as 1 plus beta T C star minus of sorry, it is I am combining this and then writing this has 1 plus beta T C star minus of T where 1 plus beta T C star is equal to T naught is beta T C.

So, essentially you know putting it in a slightly more convenient form, this whole term as 1 plus beta T C star minus of T. where, T C star is defined as this by this relationship. The advantage of looking it like this is that; given T naught and beta you know what is T C star so this is equation number I would denoted as 3, all right. So, this is we call our equation number 1 is this, tau d X d T is this. Our equation number 2 equation number 3 is this; essentially our stirred tank is described by these 2 equations, equation 3 and equation 1.

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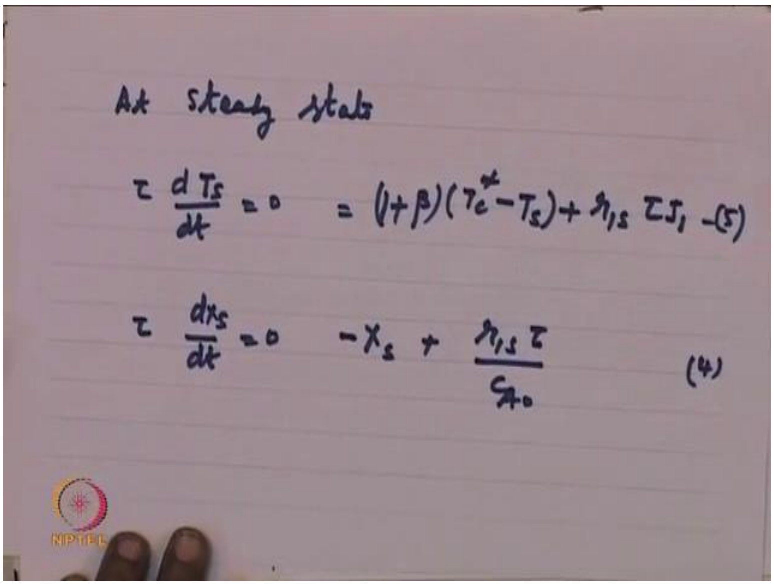

Now, what happens at steady state; at steady state we have tau d T S by d t equal to 0. Tau d X S by d t equal to 0, showing that at steady state the value of X at steady X S value of T S does not change, this is what referential steady state is all about. Therefore, that must B equal to 1 plus beta times T C star minus of T S plus r 1 S tau J 1 and then, d X S d S equal to d T equal to minus X S plus r 1 S tau divided by C A 0. So, we call this as 5, we call this as 4. Showing that steady state that you will see in our system is not described by equation 5 and equation 4.

The unsteady state is described by equation 1 and equation 2. So, that you have already said; so, equation 1 is this, equation which tells you what is the unsteady state description, and equation 2 equation 3 is this talk about temperature. So, equation 1 and 3 describe the unsteady state, equation 4 and 5 describe the steady state. Now, by stability what we means is; that the difference between the steady state number or steady state values, and the values that is the during the unsteady state, or during the period when there is some disturbance that X minus of X S, and T minus of T S. These are the variation changes from the steady state values.

We want to understand; if there is disturbance to the process what happens to this difference X minus of X S T minus of T S. In other words; you want to know whether these disturbances X minus of X S, T minus T S. Whether, they would grow and become unbounded as was the process becomes out of control. Or, they are small enough that it remains within limits that you specified, or also you would like to know; what is the trajectory of motion of a variation of disturbance from an initial point of X S and T S. So, varies things like this which you would like to know, this is what this is analysis all about which you are about ((Refer Time: 11:52)). So, we have equation 1 and 3 and then, we can have 4 and 5 describing the steady state and unsteady state. Now, what happens? Now to understand the deviation from steady state we what we do is; what is called as find you subtract equation 1 minus equation 2 and equation 3 minus of equation 5.

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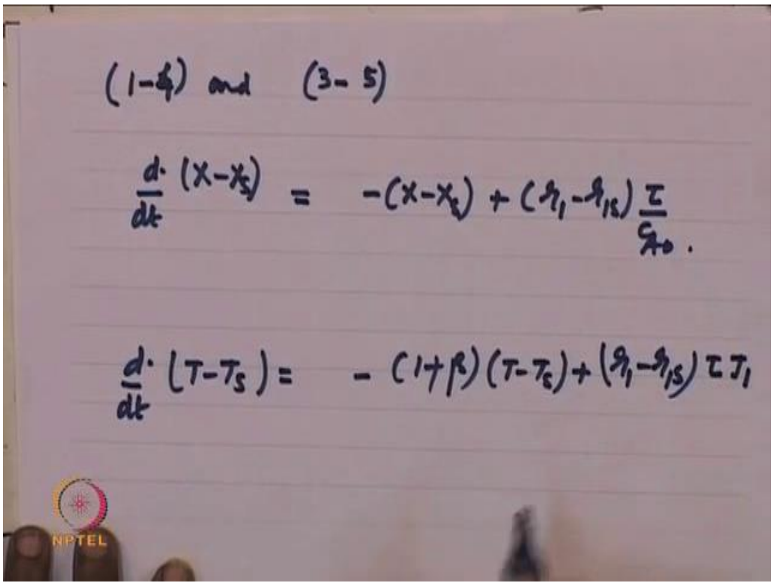

So, we do 1 minus 2 correct, 1 minus 2 is that correct; 1 minus 4, and 3 minus 5. Suppose you do this, what we get? Is d by d t of X minus of X S that is equal to minus X minus of X S plus r 1 minus of r 1 S tau by C A 0. Similarly, d by d t of T minus of T S equal to minus 1 plus beta T minus of T S plus r 1 minus of r 1 S multiplied by tau times J 1. So, what have we done? We have equation 1 and equation 3; let just run through this once again. If equation 1 which is the material balance then, we have equation 4 where is equation 4 you have equation 4; you can see here this is equation 4 and this equation 1 you can see both these equations now. Equation 1 and equation 4 so, you are doing 1 minus 4 so you get tau times d of X minus of X S minus of X minus X S and then, r 1 minus of r 1 S tau by J C A 0 multiplied. So, 1 minus 4 essentially talks about d by d T of the deviation X minus of X S, ok.

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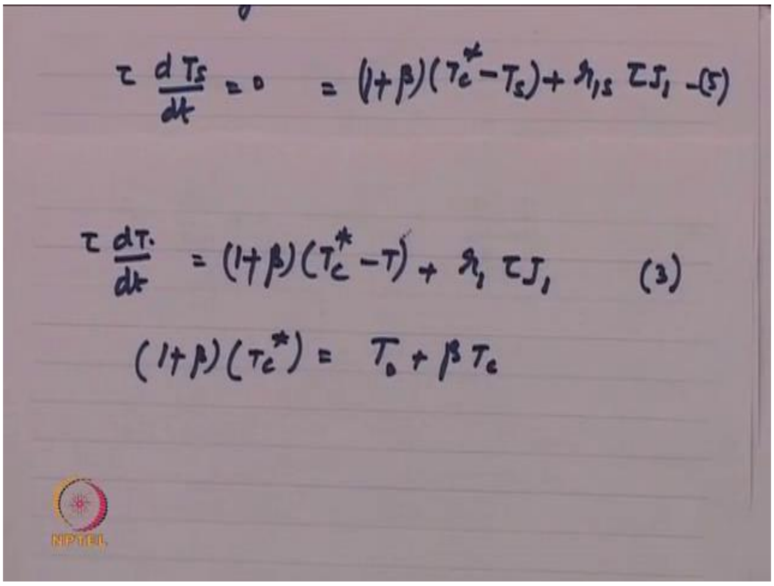

In the same way if you can look at the other one 3 and 5. So, you can look at 3 and 5; see 3 is the unsteady state, see 3 and 5; what is 3 and 5? You can see here d by d T of temperature and then, d by d T of steady state temperature so, T minus of T S you can do T minus of T S tau times. That becomes what? 1 plus beta is common, you have T C star cancels of T minus of T S with A minus sign so that is we will get it T minus of T S the minus sign. And then, we can see here r 1 J tau then, you have r 1 J tau so, will be J times tau multiplied by r 1 minus of r 1 S. So, this is what we have written here, ok.

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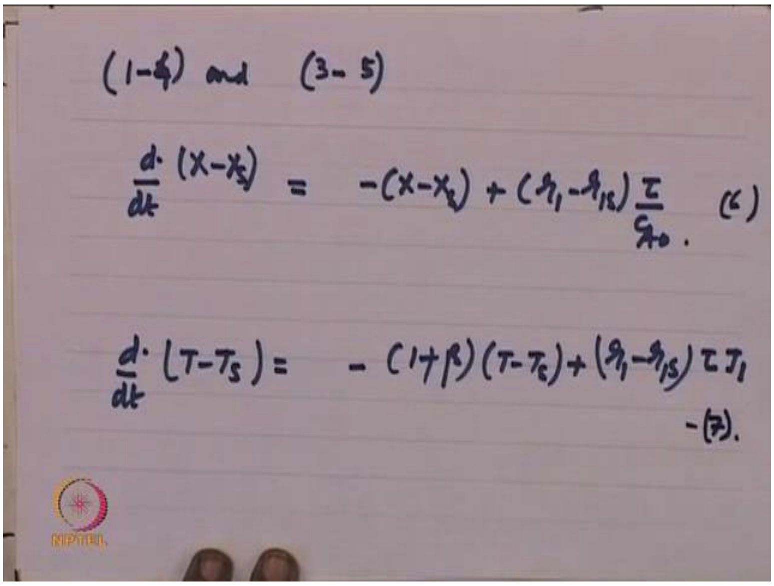

So what we have written is this so both these equations is what you have written d minus d by d t or X minus X S d by d t of T minus of T S. So, they represent the deviation from steady state. I will call this equation 6, and equation 7. Now, we want to understand what is what happens to X minus of X S with time, what happens to T minus of T S with time? Now, to be able to do this of course; since, we know the initial state we can solve then unsteady state equations using an appropriate numerical procedure and then, find out what happens. But our interest is just we get some criteria by which we can understand the system without having to go through all these mathematical calculations.

So, what we are looking at is to see whether this r 1 minus of r 1 S, this r 1 minus or r 1 S appears both the material balance and the energy balance. Whether, we can look at this difference r 1 minus of r 1 S by looking at the Taylor series expansion of this term r 1 minus of r 1 S, keeping in mind that the deviation X minus of X S and T minus of T S is not very large. In other words what we are trying to say is that; we can get an understanding of the stability of the system by doing small perturbations from the steady state. If the perturbation is very large our mathematics may not be satisfactory; we may have to do a numerical procedure to handle all these. But for small disturbance from steady state that means, X minus of X S is small, T minus T S is small, we can expand r 1 minus of r 1 S in Taylor's series and get a linear approximation to the problem.

The advantage of this procedure is that; we can get answers to our stability questions without having to solve the non-linear problems. That is the big advantage of course; how small is small? When you say X minus of X S is small, or T minus T S is small. The question of how small is small still remains is something that we will learn only we deal actual situations to make distinction between small, and how small is small. So, now what you want to do is that; we want to do what is called as linear stability analysis by linear. We mean, we will linearize this function r 1 about r 1 S and then, see what is the best estimate of r 1 minus of r 1 S we can get. So, that we can get an approximation to what happens to this unsteady state problem?

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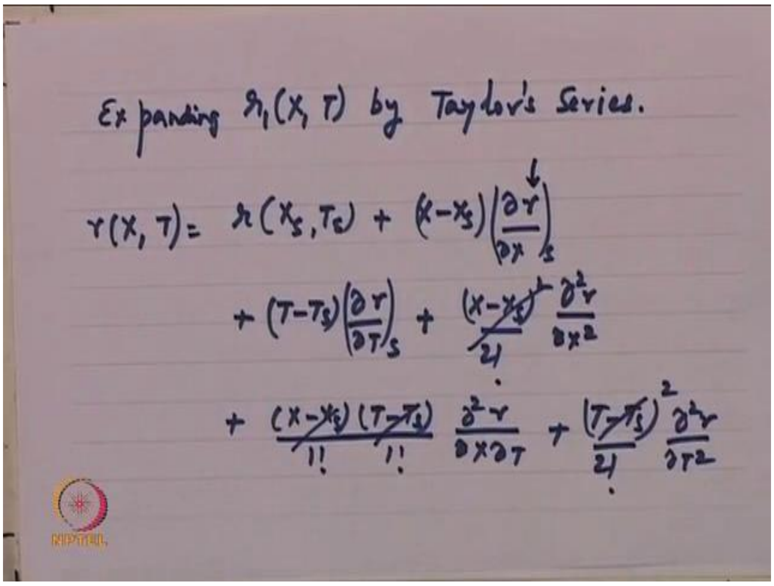

So, let us expand for example; expanding by Taylor’s series expanding r 1 at (X, T) by Taylor’s series. So, we say r of (X, T) equal to r of(X S, T S) plus X minus of X S del r by del X at S plus T minus of T S del r by del T at S, this is the first order terms. Second order terms are X minus of X S whole squared by factorial 2 del square r by del X square. Now, then we come X minus of X S, T minus of T S divided by factorial 1 factorial 1, del square r divided by del X del T plus T minus of T S whole square del square r by del T square. So, this is an expansion that we all steady at in early school so, is nothing new about this here function X T we can expand it in this way. And, so that if the second order terms or all these terms are you know very small then, we can delete this terms assuming there small.

So, that our expansion of (X T) versus about X S T as only involves X minus of X S and T minus of T S. And, therefore it is linear in X minus of X S and T minus of T S. What is del r del X steady state of del r del T at steady state, see there is rate function is known del r del X S del r del T S is also known at the steady state point. Therefore, all these can be calculated. Have you said this?

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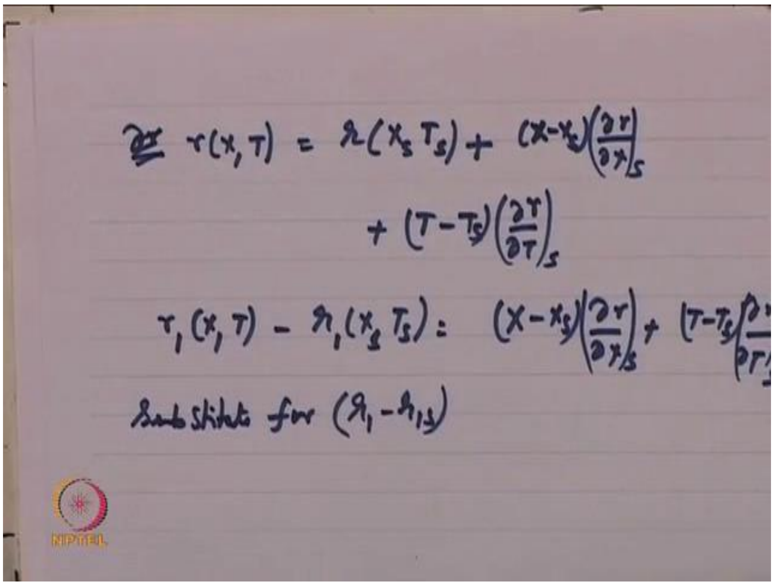

Let us see how we can so, what we are saying now is; so we have r of (X T) equal to r of(X S T S) plus you have X minus X S del r del X at S then, you have T minus of T S del r by del T at S, all right. Therefore, r 1 (X T) minus of r 1 (X s T S) is simply X minus of X S del r del X at S plus T minus of T S del r del T at S. So, what we are found here is that by Taylor's series expansion the difference between r X T and r 1 X S T X is given by this linear relationship, which is simply X minus X S multiplied by the rate of change in that direction.

Now, we can substitute for r 1 minus of r 1 S in our equations; so, we have here we notice here that our stead state the deviations from steady states given by 2 equations 6 and 7, where r 1 minus of r 1 S is occurring. Therefore, using this relationship there you are derive just now; that r of (X T) minus of r 1 at X S T has given by this relationship X S minus of X minus of X S time del r del X plus T minus T S del r del T. So, we can use that and take it forward.

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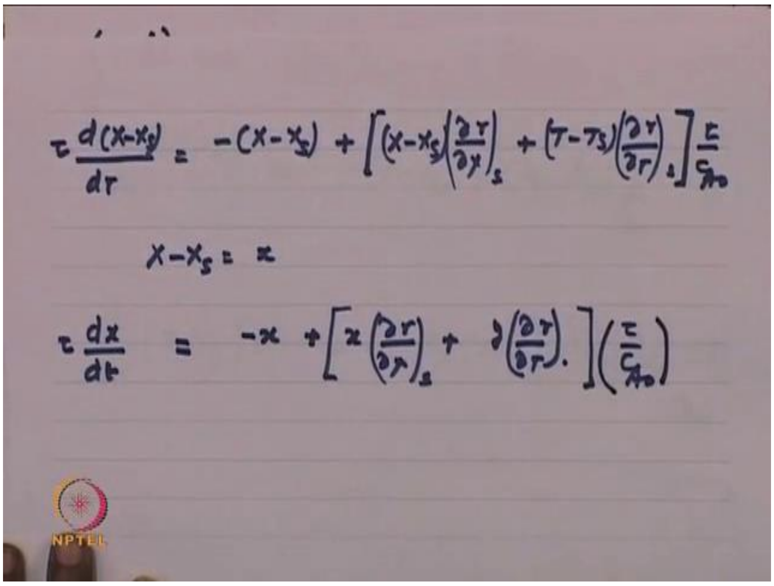

So, let us put these so our equations d by d T of X minus of X S divided by d T equal to minus of X minus of X S plus you have a r minus that is X minus of X S del r del X at S plus T minus of T S del r del T at S. What is we got here? X minus of X S del r del X is what is the term that is coming here. So, r 1 minus of r 1 S so, the right hand side we have r 1 minus of r 1 S is to replace by this equation; X minus of X S del r del X T minus of T S del r del T. Now, if I denote X minus of X S as small X; so, the left hand side becomes d X d t there is a tau here, which I have forgotten I will put it again.

Now, that is equal to first term is minus of X. The second term is what? Plus X del r del X at S then, plus y del r del T. And, what is our equation, where is our equation here? Our equation is r 1 minus of it multiplied by tau C A 0. So, we will have to multiply r 1 minus of r 1 S r 1 minus this whole term should be multiplied by tau by C A 0. So, this is also we should multiply by tau by C A 0. I hope we understand what I am saying. Let us see go through once again so that there is no confusion. What we have done? We have expressed in the form of a differential equation X minus of X S and T minus of T S.

The right hand side they involve a term r 1 minus of r 1 S in both material balance and energy balance. Then, we said that r 1 minus of r 1 S this can be understood from looking at the Taylor’s series expansion for function r times r X, which we are done here. so, this gives as r X T minus of r 1 X S T S suppose that difference between r 1 and r 1 S, it is given by this relationship X minus of X S del r del X and T minus of T S del r del T, ok.

So we have to substitute for that here; therefore, r 1 minus of r 1 S has to be multiplied by tau by J C A 0, this what we have done here. So, our relationship for the variation of X with time is given by this relationship, which involves all the terms that we have talked about. Now, let us do the same thing energy balance.

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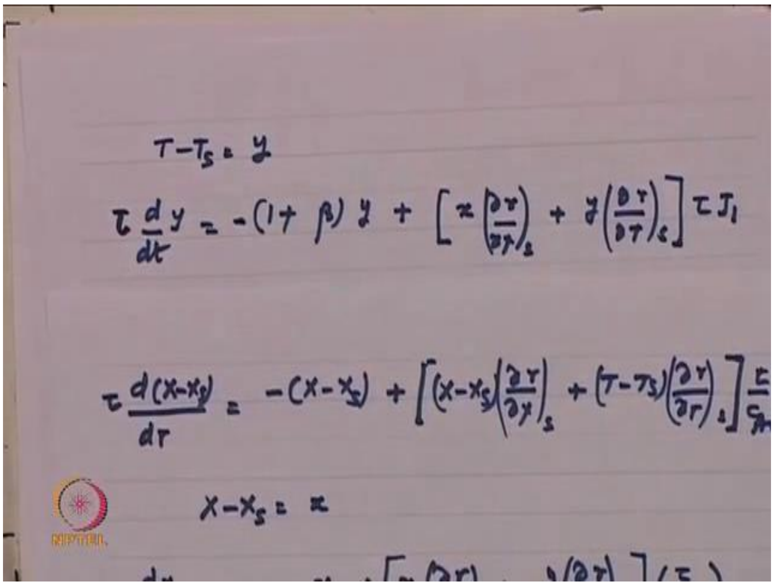

What is our energy balance? So, we are doing the same thing for energy balance. So, we say tau where are we, see equation 7 is our energy balance so, which I am writing it as T minus of T S let us say is y. So, become d by d T of y equal to 1 plus beta T minus of T S is y, plus this is r 1 minus of r 1 S let me write it down in the form in which we want. Which is within brackets of X minus of X which is x del r del X at S plus y T minus del r del T at S, is that clear. So, our balance now looks like so, this is r 1 minus of r 1 S you have to multiply by tau times J 1. So, we have 2 equations now; so, we have the material balance equation giving you tau d X d T equal to on the right hand side, and you have the energy balance equation giving you equation of the form d y d t of 1 plus beta and so on. And, then this 1 plus beta must have a negative sign I have forgot the negative sign, all right. So, we have these 2 equations tau d X d T equal to this, and d y d t tau is missing here, ok.

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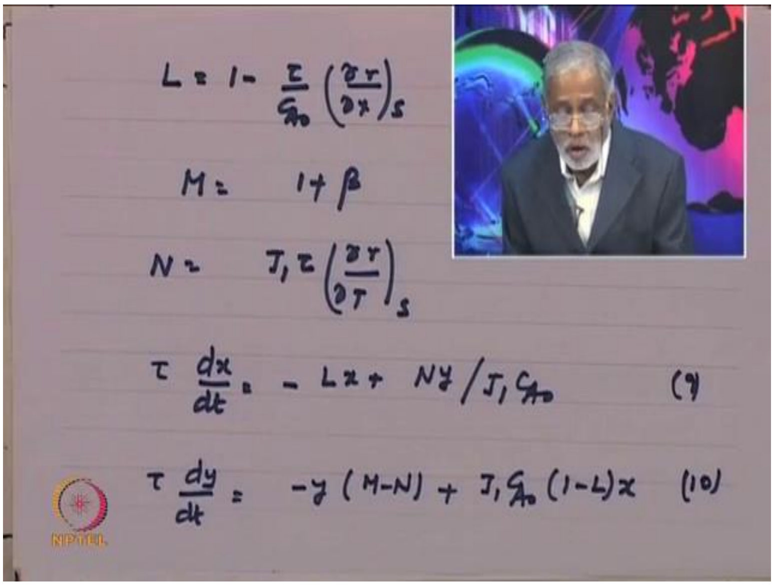

Now we can put this in a nice form; is taken from rather for dialysis book, and the forms in which these equations are available I try the final forms because these are not very difficult to do, these are all available in this form in the lit. So, what we are saying is that the differential equations that is with us to be solved in the literature. It is available in terms of L M and N. Where, L is defined like this, M is define like this, N is define like this. So, that our equation tau d x d t can be written like this N y divided by J 1 C A 0 and tau d y d t equal to minus of y times M minus of N plus J 1 C A 0 1 minus of L times x. So, I mean you might ask how I got this is some very elementary manipulation, you have to put all these things in terms of L M and N. In simplify these 2 equations and it is nothing very complicated it will come very nicely.

So, what I saying what we are saying now is that x and y represent the deviation from steady state. And then, this differential equation I will call it equation 7 8 9 10. Let us say it is 9 10 these equations 9 and 10 describe how x and y change with time as the process is disturb because of some external disturbances. So, our interest is now to solve this, of course; this can be solving numerically that is not a big problem. But we can get answer to this by looking at the matrix of the variations that we have talked about. Let us do that now.

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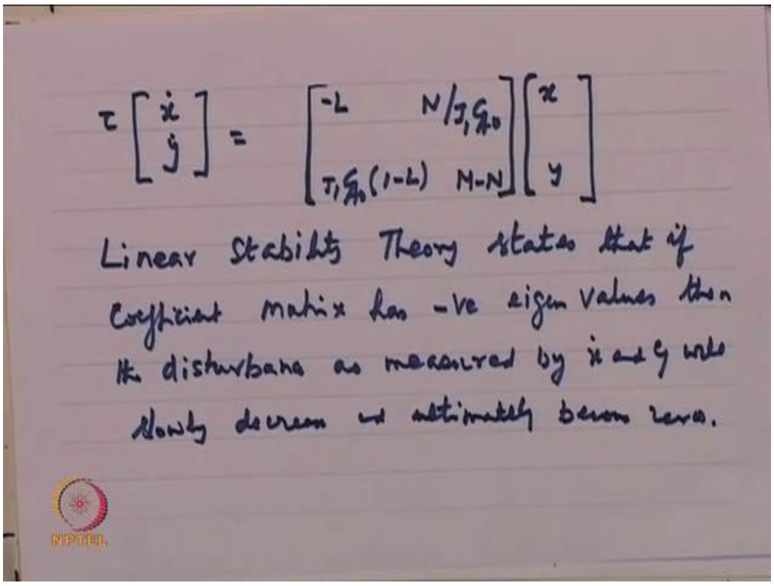

So, let us represent this equation tau within brackets of x dot and y dot. What is the x dot and y dot? x dot is d x by d t, y dot is d y by d t, x represents deviation in conversion, y represent deviation in temperature which respect to steady state. So, in this form we can write our matrix, which is X and y so, this matrix looks like this. So, it is minus of L N by J 1 C A 0 J 1 C A 0 times L minus of L M minus of N. So, this is fairly straight forward, this is nothing much in it. So, this is just written in the matrix form that is all. X dot y dot represent d y d t and d x d t and then, x and y taken common in all that you will get, what you are say.

Now, if we have a matrix differential equation whether, coefficient matrix here consists of terms which are constant. So, the coefficiences L M and N they are all constant. Therefore, this coefficient matrix tells us something about the system which is undergoing a transient change. The linear stability theory says, linear stability theory states that; if coefficient matrix has negative Eigen values then, the disturbance as measured by x dot and y dot will slowly decrease, and ultimately become 0. What are we saying? What are we saying is that the Eigen values are negative then, the disturbance x dot x and y will slowly die, and eventually it will reaches the previous steady state from where it started, ok.

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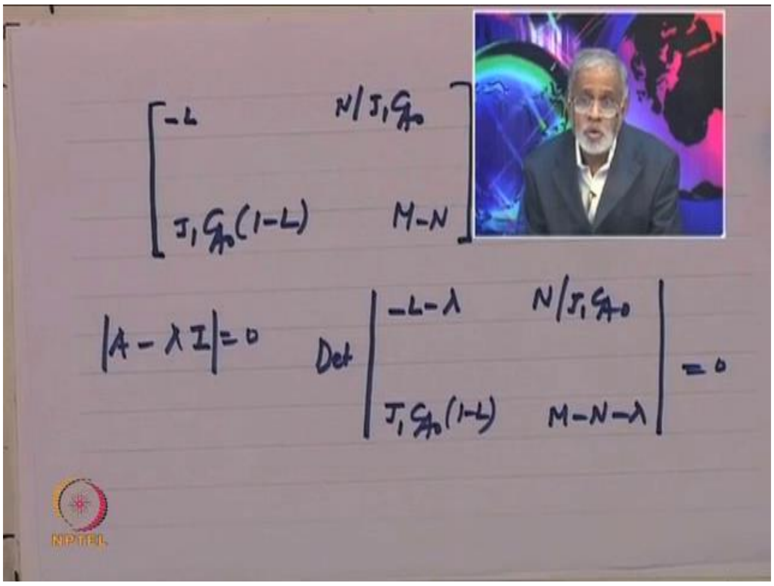

Now, how do you impose the condition that; these values of the Eigen values are negative suppose you want to make the Eigen values negative that means; what is the condition that we can impose. The condition that we can impose is; that if you have a matrix which is minus of L N by J 1 C A 0 J 1 C A 0 times 1 minus of L M minus of N this matrix must have negative Eigen values. How do you find that means; how do you find the Eigen values of a matrix A minus of lambda I equal to 0. That determinant tells you the so you have to find the determinant I will say determinant of minus of L minus of lambda N by J 1 C A 0 M minus of N minus of lambda. So, this determinant what goes to 0? So, this must be equal to 0.

Then, these Eigen values should become negative, or if it is complex the real part must be negative. If that is a case then the disturbance that is measured by x dot and y dot tend to become smaller and smaller, and in long period of time completely disappear. So, our criteria for stability of our steady state are that Eigen values of this matrix must be negative. So, how do we what how do impose that condition on this matrix that condition we impose on this matrix is that the determinant must have negative Eigen values.

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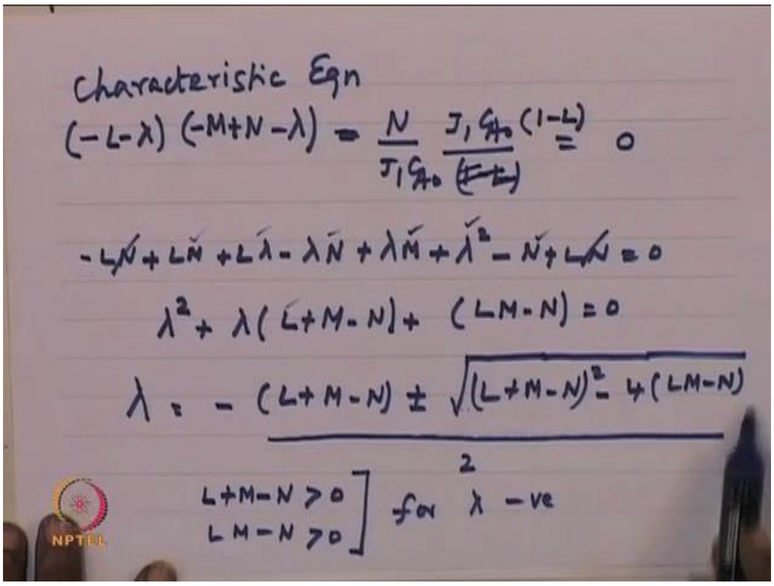

So, let us find the determinant so, you have minus of lambda so, we have I am writing the determinant please. If it is so, minus of L minus of lambda multiplied by M minus of N minus of lambda equal to N by sorry, minus J 1 C A 0 J 1 C A 0 divided by 1 minus of L. This must be equal to determinant must be equal to 0. What are we saying to find the Eigen values we will have to say A minus of lambda A equal to 0. That is what we have done so that A minus of lambda A equal to 0 specifies; that this characteristic equation this is the characteristic equation must be 0.

So, this tells us what are the values of lambda? Let us solve this so, when we solve this let me write down minus of L N plus L N plus L lambda minus of lambda N plus lambda M plus lambda square minus of N plus L N equal to 0. This is minus sign here, which I notice it is minus lambda. So, it is minus M plus N that is why fine. See I have put it on the numerator so, 1 minus I am sorry, that is why J 1 C A 0 1 minus of L divided by N by J 1 C A 0 that is better, ok.

So, this is correct so we can simplify this, and write this as our characteristic equation looks like this. Lambda square plus lambda times L plus M minus of N plus within bracket L M minus of N equal to 0. L M minus of is it correct, L M minus of N, L M some terms. So, lambda square so this is correct, lambda square L M L M minus of N this term is taken. Now, lambda times L lambda so, this term is taken minus of lambda N this sorry, this term is taken, this term is taken. And then, L lambda N this term is taken. So, all the term have taken so only term is these 2 cancels off, this is fine.

Therefore, solution is minus L M L plus M minus of N plus or minus of root of L plus M minus of N whole squared minus of 4 times L M minus of N divided by 2. So, this is the Eigen value, and we must put the condition that these Eigen values are negative. Now, if it turn out to be complex the real part must be negative. So, this is the condition that you must impose. And then, it stands to reason simply to recognize that L plus M minus of N must be greater than 0, and L M minus of N greater than 0. So, for lambda negative; that is just understood whether, this is satisfactory from our first principles.

You want lambda to be negative, when we lambda to be negative the left hand side L plus M minus of N must be greater than 0. So, the this term is always negative, and the term inside L plus M minus of N so, this must be L plus M minus of N must be this whole thing has to be; such that you see if you make L M minus of N greater than 0. So, this is greater than 0 you find the whole term becomes less than N plus M minus of N. Therefore, although both the roots become negative this is what we have to recognize. You want to both the roots to be negative so, this nice condition L plus M minus of N is greater than 0, L M minus of N greater than 0.

So, there could be situation when the second term is very large compare with the first one. So, that the whole terms becomes what is called as complex so, movement becomes imaginary the second term which means what? The real term Eigen values the real part is negative. But it has A complex part which only means that is an oscillation involved in the process.

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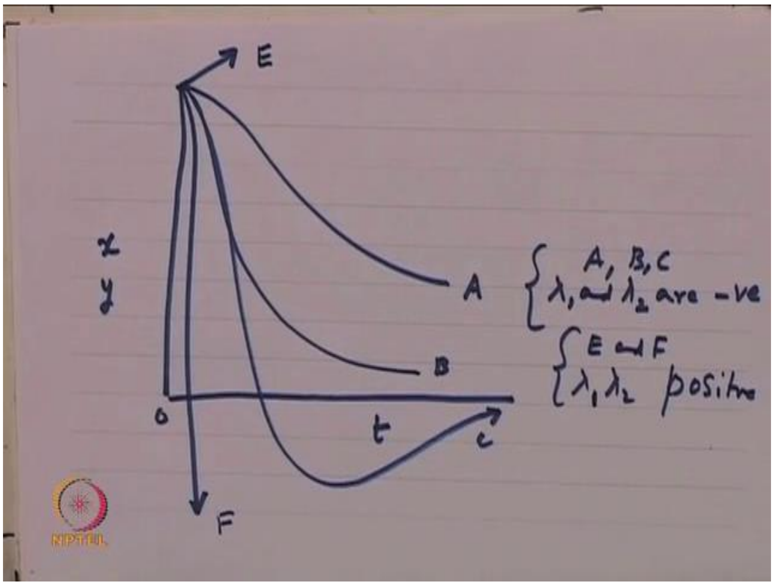

Now, just quickly look at what we are saying; what are we saying is we have time of x or y let us say. So, this is an instance when lambda 1 and lambda 2 are negative so, when lambda 1 and lambda 2 are both negative. What you find is that; this both x and y this is 0 so, it is start with some value. It starts to d k and it takes certain amount of time to become 0. Now, this can also be like this, or this can also be like this. So, A B C so the instances of A B C are 3 types of values of lambda 1 and lambda 2. But such that there all because lambda 1 and lambda 2 are negative, the deviation x and y goes to 0 in various ways. But these are all instantiates of stable steady state, because both x and y become 0 in infinite time. That is a meaning of a asymptotic stability, ok.

So, there could be instants where in a it sort of runs away. So, this E and F are values of lambda 1 and lambdas 2 are positive. So, this is E and F when lambda 1 and lambda 2 are positive, the process runs away which means that there are instances of unstable situation that means there is a disturbance under condition E and F. It does not return to the same stead state, therefore; instances there are unstable, ok. Let us look at one more instance; what is that instance is when the lambda has a complex? That means, the lambda has complex which means there is a real part, but there is an imaginary part as a result of which there is oscillation.

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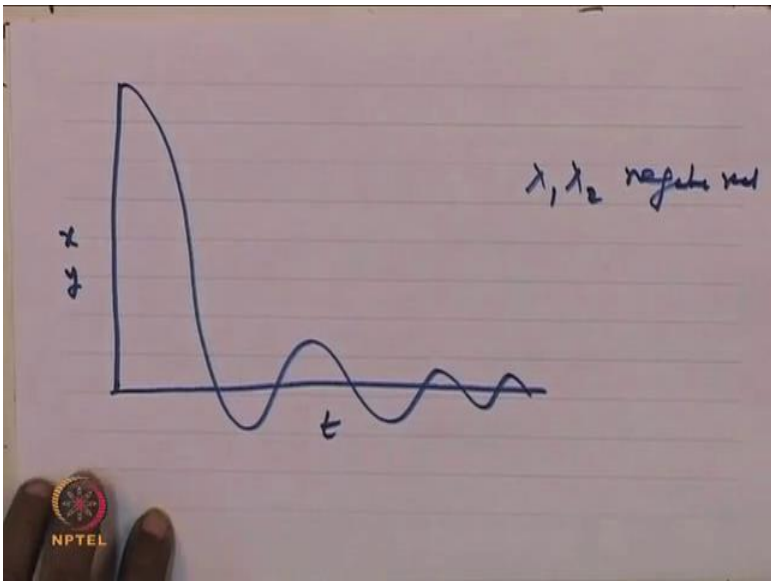

So, there are two types of oscillations. So, time x and y what we are saying is that; there is negative real part, but there is oscillation, which means; what you have that means it oscillates see as, but because of the lambda is negative real lambda 1 and lambda 2 are negative real part is negative real. So, that the complex part starts to d k.

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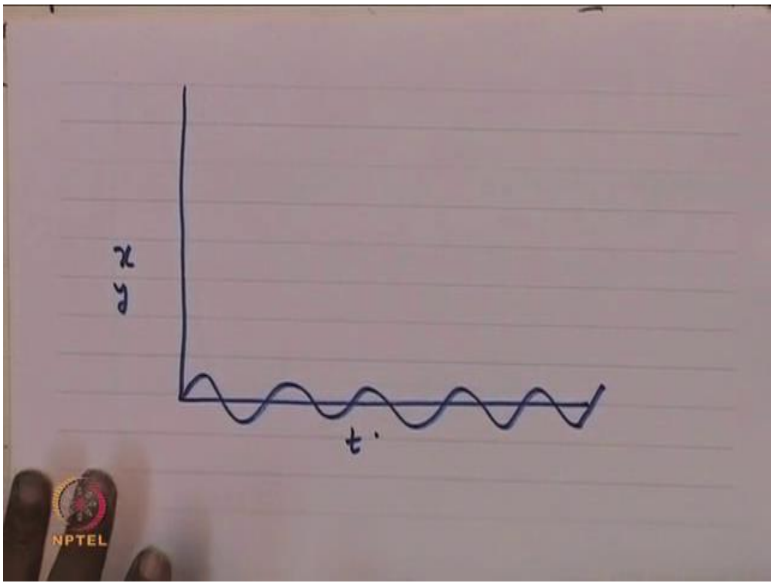

So there is one more instance you will see that is; you have lambda 1 lambda 2 are 0. The real part is 0 and then, the imaginary the other part is complex showing that you see you can have what is called as a stable oscillation. It is stable oscillation, when the real part is 0 there is a complex part which means the stable oscillation. Stable oscillation can be seen as a steady as long as the oscillations are within the limits that you would specify. So, what we have done is that we have formulated the problem in terms of deviation from steady state. You have looked at how to make these deviations the Eigen values of this matrix should be negative real. You put the conditions for that we say the conditions are L plus M minus of N greater than 0, L M minus of N equal to greater than 0. These 2 conditions are satisfied the steady state is stable, provided the lambdas have negative real part, ok.

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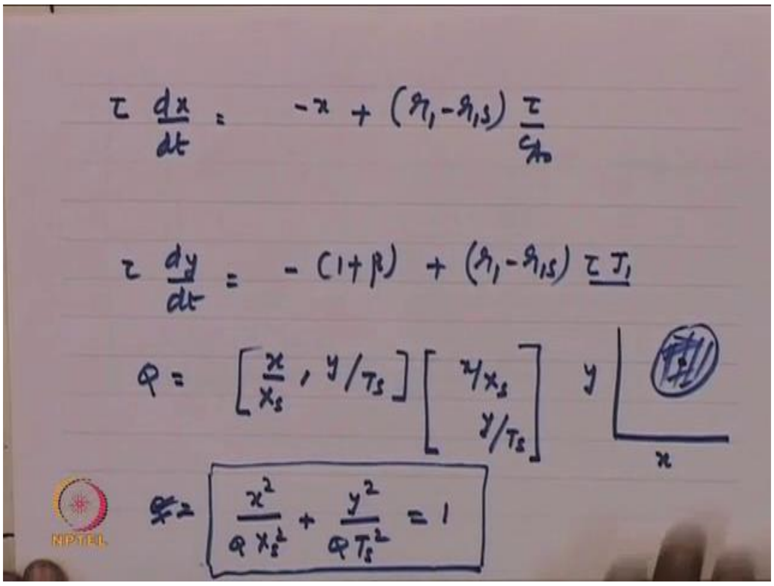

Now, there is another way by which we can look at all this. Let us do this quickly. So, what we are saying is that; let us just write down the equation once again, our equation is d x d t equal to minus of x plus r 1 minus of r 1 S tau by C A 0. Tau d y d t is minus of 1 plus beta plus r 1 minus of r 1 S multiplied by tau J 1 by J 1, is that clear. You want to understand stability in the context of a process. Now, in a process our variables x which is deviation from steady state, variable y which is deviation from steady state in temperature, all these will change. It will not be at the steady state that you want I have specified. Therefore, when you run A process we accept certain variations. Now, within the limits if these variations are within limits that we specify, we have still willing to except. So, suppose I say that Q equal to x by X S comma y by T S, ok.

Suppose, I define a quadratic form which is x by X S comma y by multiplied by this vector so, or what we are saying is that x squared by X S square, and y squared by T S square equal to some number. Suppose I say that as long as this Q is within my limits I am willing to except the process. Suppose, we do that what it means, what it means is that; if I expand this Q equal to x squared by Q X S square plus y square by Q T S square equal to 1. So, if I put this in this form that means; I can suppose I say that in my process I am willing to except Q as the value of the objective. What is that objective that x by X S comma, y by T S this quadratic form should be equal to Q at best or, express in this form. This ellipse this is the equation to an ellipse, suppose I make a plot of y and x. So, I get in ellipse, and this is the point of steady state as long as my x and y stay within this ellipse, I am willing to except the process.

So, on other words; what we are trying to say by looking at the stability analysis of an exothermic stirred tank is that x and y will change. It will change depending upon how well we run the process, but if we define a quadratic form. And, if you can run the process within that ellipse; we are willing to except and say that it is a stable process. We are willing to except what over variations and this is 1 way of trying to run a process, because it is very difficult to keep the values of x and y at the points why you would like.

Thank you very much.