Chemical Reaction Engineering

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Lecture No. # 37

Stability Analysis - Examples

Friends, let us continue our discussion on stability of chemical reactors and in the today's class, we will look at specific examples to see how we determine the stability and what implications does it have? To recap, what we saw in the last session.

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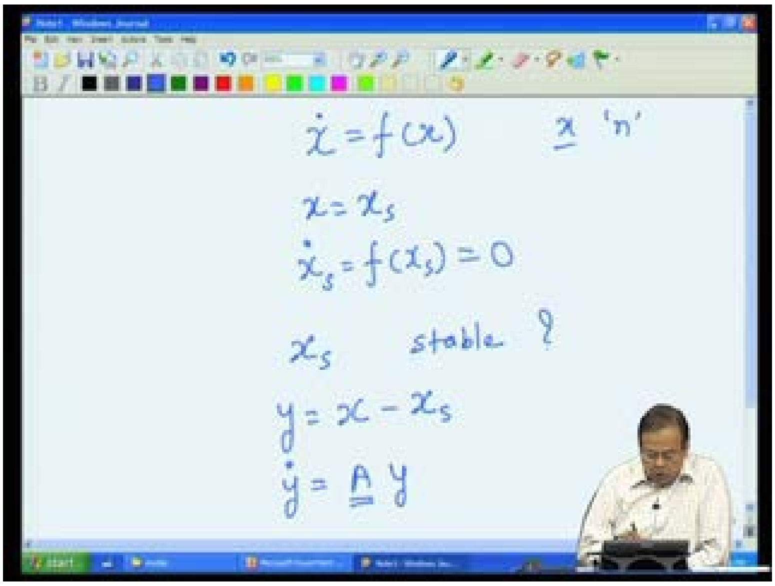

We have the dynamics of our system being described by x dot equal to f of x, where x is a vector of n dimensional space. And we want to find out, if x equal to x(s) is the steady state solution of this system; it means that, x s dot which is f of x s is 0; that is what we mean by a steady state solution. So, we are interested in knowing whether the steady state solution x s that we get, is it stable or otherwise; we defined formally what stability stability means. So, we are looking at solutions which are asymptotically stable. And for this by doing a linearized analysis; that is linearizing the dynamics around this steady state and describing the perturbation that is the perturbation from the steady state and its dynamics such that y dot is equal to A y.

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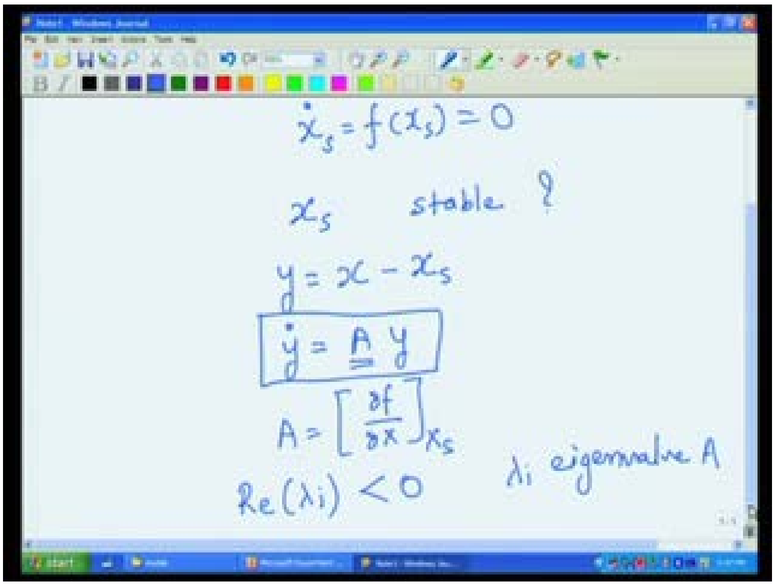

Where A is a Jacobian matrix del f del x evaluated at x s and we know the solution of this linear equation is in terms of its Eigen values. And therefore, we said the condition for the steady state x s to be stable is that real value of Eigen value real part of the Eigen value should be less than 0; where lambda i is the Eigen value of the matrix Jacobian matrix A. If it is if it is one of them is positive, then the system is unstable and if the real part is 0, we cannot say much about the stability of this system. So, now let us take the example to see how we determine this determine this stability.

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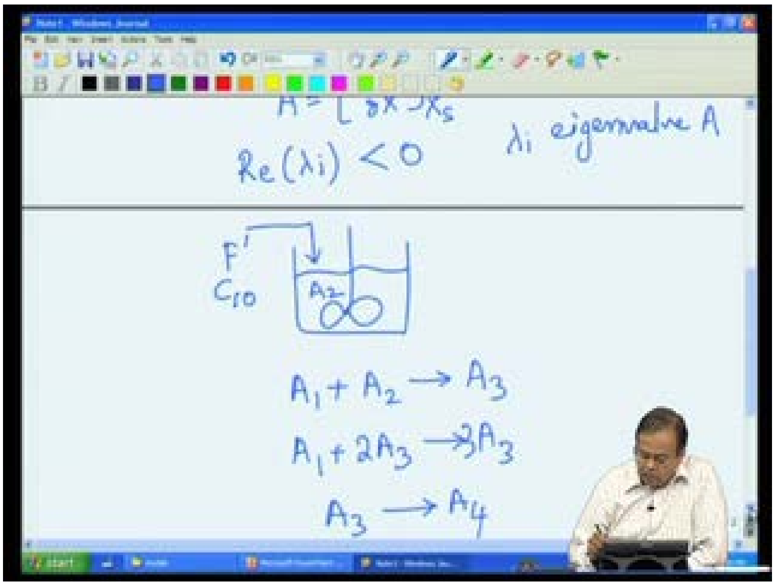

So, let us say that we have a stirred tank reactor, which is operated in a semi batch mode. So, we are feeding in some feed which in this particular case consist of the component 1 at some concentration. And the reactions that we are interested in or reaction that are taking place is A 1 plus A 2 gives rise to A 3. Then, A 1 plus 2 A 3 gives rise to 3 A 3 and A 3 gives rise to A 4. This is an example of an autocatalytic reaction. So, we would like to do some stability analysis for this. So, for this reaction we are we are providing A 1; there is lot of A 2 in the reactor lot of A 2 in the reactor and we are continuously adding A 1 that is our that is our system. So, let us let us try to write the dynamic equations or mass balances for this. I am going to consider an isothermal system. Our non-isothermal example will come little little later on.

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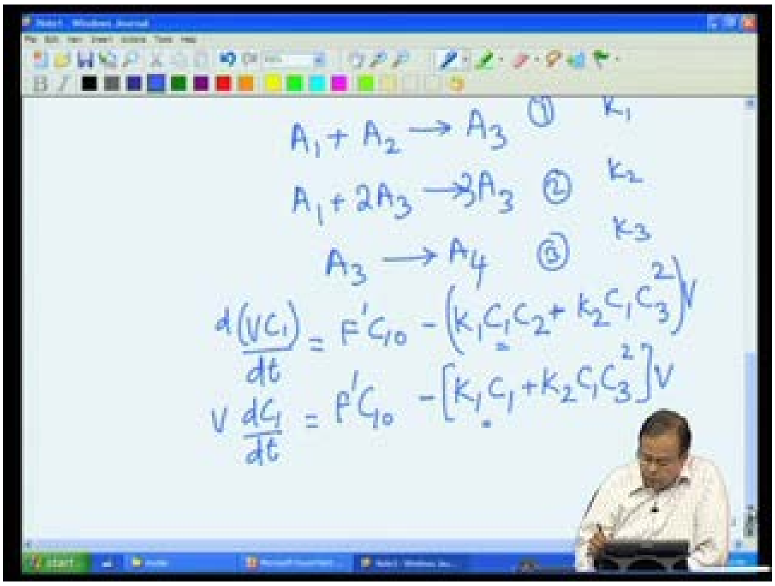

So, let us try to write the mass balance for this. Starting with component 1, now what is happening to component 1? Component 1, we have A being fed in to the reactor. So, if we actually write, let me start from the beginning. If we actually write the mass balance for the total amount of amount of A 1, so mole balance or mass balance; So, C 1 is the concentration times the volume is the moles or mass. So, the rate of its accumulation must be equal to the rate at which material is being fed namely F 1 F prime in to C 10 minus the rate at which it is getting consumed. So, A 1 is getting consumed in first two reactions. So, let us call these reactions as 1, 2 and 3 and corresponding rate constants as K 1, K 2 and K 3. So, what will we have?

We will have minus K 1 C 1 C 2 and minus K 2 C 1 C 3 square representing the three reactions that we that we have. Now, ofcourse this let us put this in to the volume; because our reaction rates are in terms of intrinsic rate per unit volume and since we are doing doing a mass balance on the component, now here we are going to make certain certain simplification. So, that our our analysis remains manageable. The first thing we are going to assume is we are going to have lot of A 2 in the reactor to begin with with large volume. So, when you add some little bit of A 1, first we will assume that volume is not going to change significantly. And second we will assume that since concentration of our A 2 is present in large quantities, its concentration is large.

Our reaction first reaction that we wrote is a pseudo first order reaction; that means firstly I am going to assume that volume is fairly constant. So, I will just take out volume out and write dC 1 dt V into dC 1 dt equal to F prime C 10 minus… I am going to absorb this C 2 in the assumption that concentration of species 2 is very large compared to all other species. So, its variation is negligible. I am going to absorb that into rate constant and just going to call this reaction as pseudo first order first order reaction. So, although I am calling it same constant K 1 between this step to this step, I have just absorbed this concentration K 1 C C 2 in to in to K 1 and then we have K 2 in to C 1 C 3 square in to V; this, I am going to simplify little bit this mass balance.

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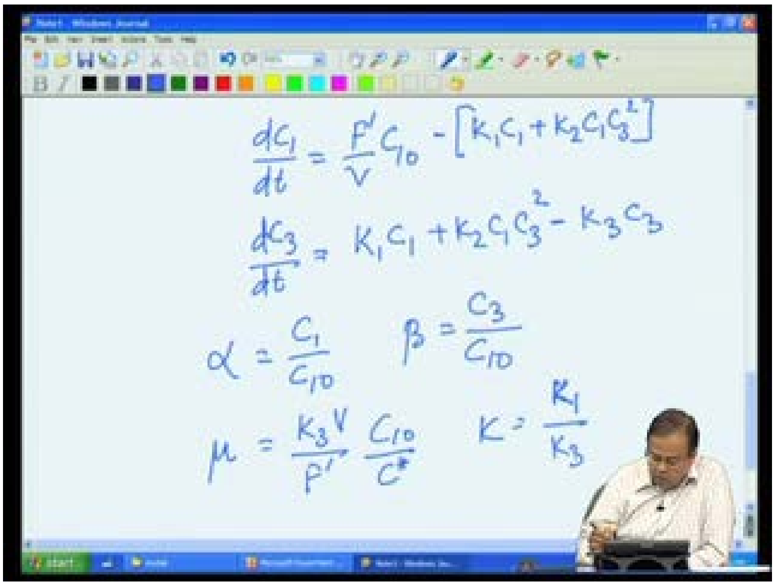

And therefore, then write dC 1 dt equal to F prime by V in to C 1 naught minus K 1 C 1 plus K 2 C 1 C 3 square; that is my mass balance for species 1. And with the same assumption, I can write my mass balance for species 3; because species 2, I am assuming that its concentration variation is negligibly negligibly small. So, what is happening to species 3? Species 3 is getting formed in in in reaction reaction 1. It is getting consumed or rather formed in reaction 2; because it is getting consumed as well as formed. But stochiometry suggests that it is formed in excess of what is getting consumed and it is getting consumed in third reaction. So, if I do the proper mass balance for this now, I can I can write now there is no feeding of species 3.

So, I can straightaway write it is getting produced in reaction 1 and 2 and getting consumed in reaction 3. So, these two quantities are now sufficient for me to describe the dynamics of the whole system; because if you look at C 4, it will be simply K 3 in to C 3. So, I need not worry about C 4 in my in my analysis. So, we now have we now have our mass balance equations, which once again for sake of sake of simplicity; I am going to make these equations dimensionless. By defining my dimensionless concentration, let us say let us say alpha as C 10 sorry C 1 by C 10; beta as dimensionless concentration of species 3 by C 10. Then, few more quantities mu equal to K 3 V by F prime in to C 10 by C star and kappa as rate constant K 1 by K 3. And if you do all that and substitute this in the dimensionless dimensionless quantities, by the way, what is C star?

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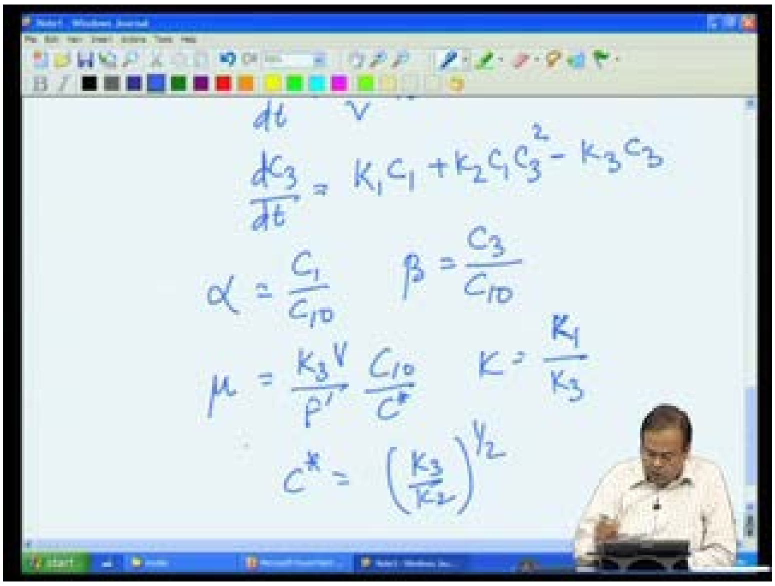

C star is K 3 by K 2 raise to half. So, if I if I take my mass balance equations, use these dimensionless quantities; I can write my I can write my mass balance equations as as follows.

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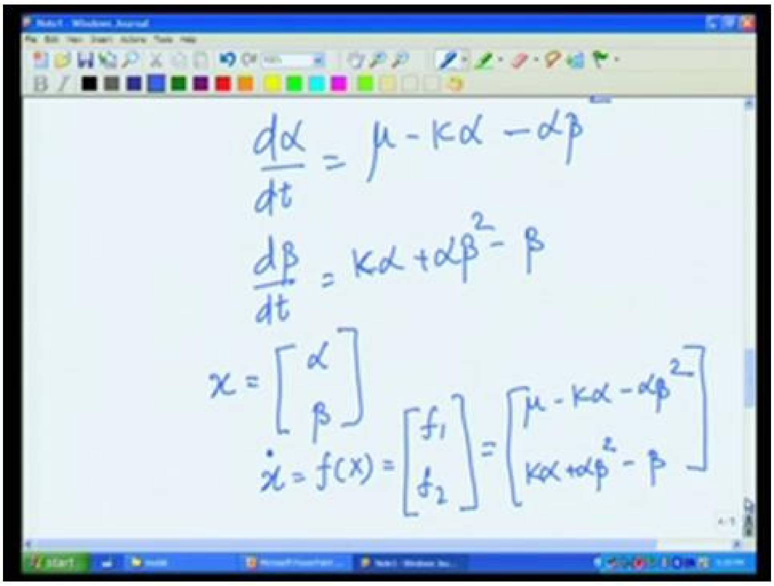

(No audio from 12:35 to 13:05) So, I can write these mass balance equations in in in terms of these dimensionless dimensionless quantities, where this kappa is everything is defined in the previous previous slide. So, now what I have? Now, what I have is my dimensional mass balances made dimensionless by defining these these quantities which convert my dimensional mass balance equations to dimensionless dimensionless form. Now, I want to look at the steady state of this. So, now let us let us try to try to map it with whatever general formulation that we have. So, let us first define our state vector which is our alpha and beta. Now, its dynamics its dynamics x dot is equal to f of x. We will have now two components f 1 and f 2 which are according to these mass balances; mu minus kappa alpha minus alpha beta square, which is my f 1 and kappa alpha plus alpha beta square minus beta, which is my f 2. So, now I have defined my f 1 and f 2. So, I need to define my steady state now.

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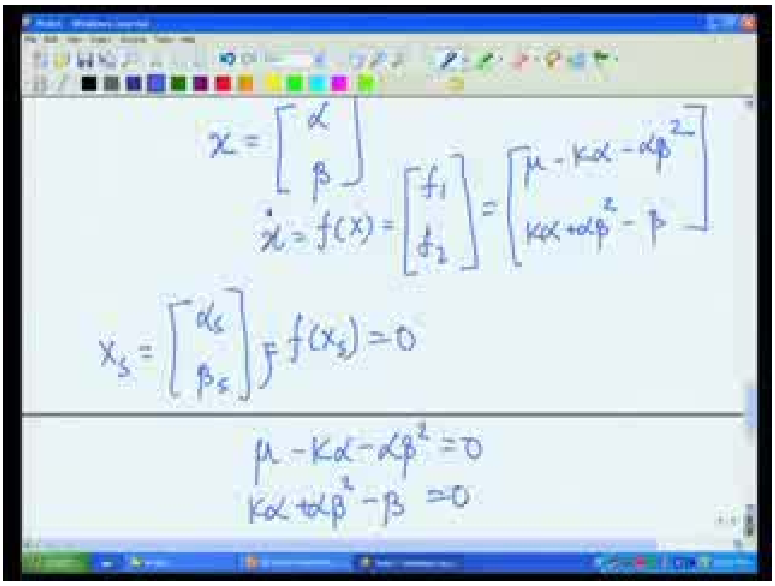

So, what is my x s? That is alpha steady state and beta steady state. This is given by f of x s equal to 0; that means, mu minus kappa alpha minus alpha beta square equal to 0. My f 1 equal to 0 and kappa alpha plus alpha beta square minus beta equal to 0 right.

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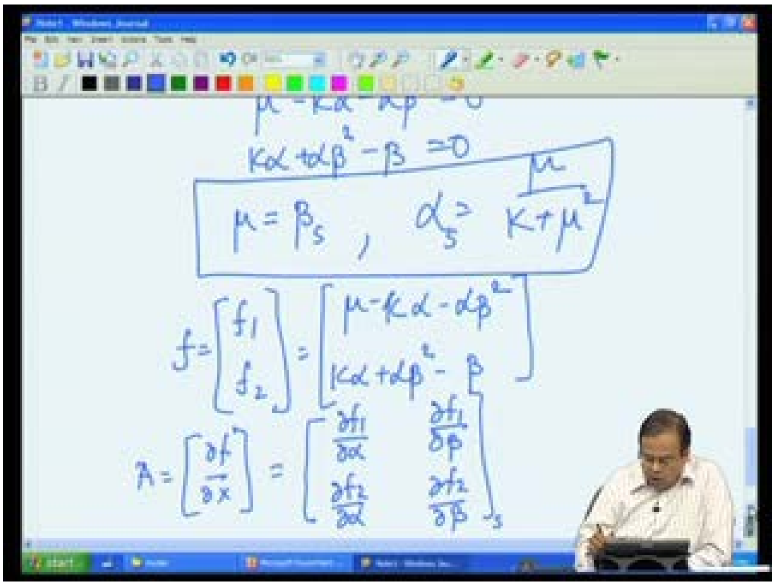

So, if you look at these two So, if you look at these two solutions, first I get my if I add these two for example; I will simply get mu is equal to beta or that is our steady state solution beta s. And if I substitute the value of beta s over here, then I will get my my alpha. That is, if I substitute for beta s equal to mu, I will get mu by kappa plus mu square is my steady state solution alpha s and beta s. So, this is my steady state solution. And I would like to know, whether this steady state is a stable steady state or unstable or whatever is the status of that steady state. As you can see here, it will depend upon the values of mu and kappa and so on.

So, let us try to do some some analysis. So, let me let me rewrite my f, which is f 1 and f 2; which is mu minus kappa alpha minus alpha beta square and kappa alpha plus alpha beta square minus beta. I need to find the Jacobian matrix now. What is my Jacobin matrix? My Jacobian matrix is del f del x; that means in this particular case, I can write it as del f 1 del alpha. Because my x is nothing but alpha and beta and del f 1 del beta, del f 2 del alpha and del f 2 del beta. So, this is my this is my Jacobian; all evaluated at steady state. So, what is what is what is let us let us put these let us put these quantities quantities of del alpha and and and and so on. So, what is our first term?

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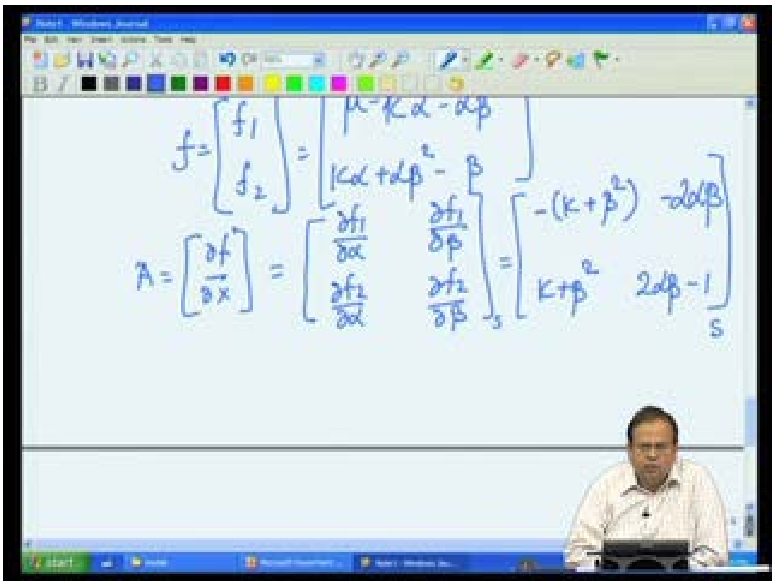

I am just going to put it over here; del f 1, this is my f 1 by del alpha. So, that will be simply minus kappa plus beta square; that is the first term; then del alpha del beta del f 1 del beta. So, what will be that? That will be partial derivative of this f 1 is nothing but 2 alpha beta; then the second term f 2 and del f 2 del f 1. So, del alpha sorry del f 2 del alpha. So, that will be just kappa plus beta square and del f 2 del beta, which will be 2 alpha beta minus 1. All evaluated at the steady state value that is alpha equal to alpha s and beta equal to beta s.

So, for this example, we now have our our Jacobin matrix with specified values of alpha s and beta s. So, we need to find out whether that Eigen values will have real part or positive real part or negative real part and so on. But since this is a two-dimensional system, we had only two state variables, alpha and beta. Let us try to do some analysis to the extent that is possible. We cannot determine the values of Eigen values probably that easily ofcourse you know for a 2 by 2 system; you can actually find out analytically.

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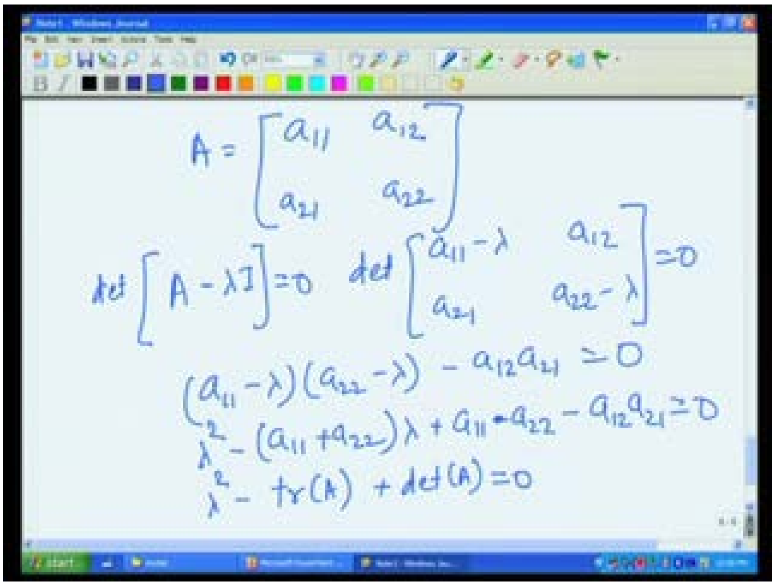

But let us let us try to then write this matrix A in a general form as a 11 a 12 a 21 a 22 and try to try to determine the Eigen values of this particular particular matrix; So that, we can say something about about the behavior of this of this system. So, what is the Eigen value? Eigen value is nothing but determinant A minus lambda I equal to 0 or determinant a 11 minus lambda a 12 a 21 a 22 minus lambda equal to 0. And for a two-dimensional system, for two-dimensional dimensional system we actually can write therefore a 11 minus lambda in to a 22 minus lambda; just determinant by of two by two system, minus a 12 a 21 equal to equal to 0; which on further simplification gives us lambda square minus a 11 plus a 22 in to lambda plus a 11 minus a 11 in to a 22 minus a 12 a 21 equal to 0.

I am just expanding this algebraic algebraic equation. Now, if we examine these terms individually, what is a 11 and a 22? a 11 plus a 22 rather? In terms of determinants on matrices that is nothing but trace of this matrix A or let us let us trace is just the diagonal element addition. So, let us let us write it in a proper proper notation. We can write this as trace of A and what is a 11 a 22 minus a 12 a 21? That is just nothing but determinant of matrix A. So, my Eigen values are satisfying this equation lambda square minus trace A lambda plus determinant A equal to equal to 0 is a quadratic equation. So, we know the analytical solution to this quadratic equation.

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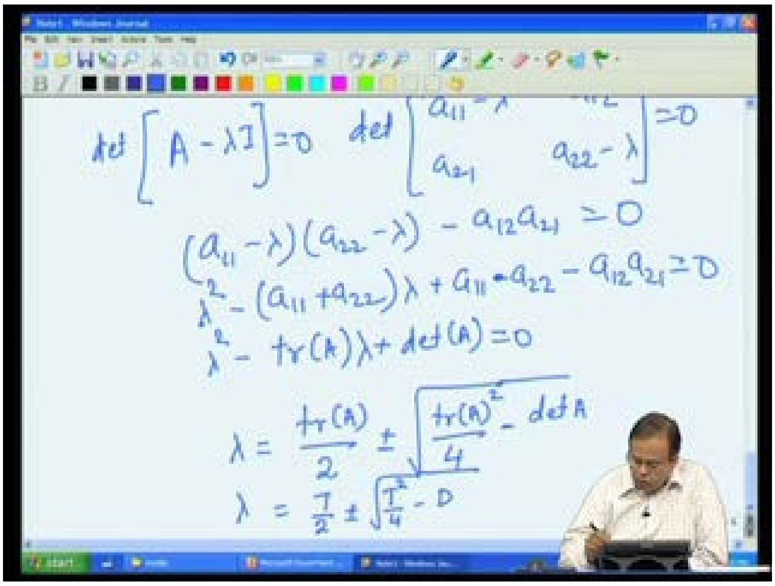

So, that is lambda is trace A by 2 plus or minus or if you write it in a plus or minus square root of trace A the whole square divided by 4 minus determinant A; that is a solution of a that is a solution of a quadratic quadratic equation. Let us write trace A as T. So, this is T by 2 plus or minus square root of T square by 4 minus D, where I am writing T for trace A and D for determinant or in other words, whether for a 2 by 2 system, I know my Eigen values analytically. So, all I need to do is calculate trace, calculate determinants, substitute these values and I will know my know my trace and determinant. If I know my trace and determinant, I know my Eigen value.

So, if I know my Eigen value, I can I can write; I can determine whether my steady state is stable or otherwise. But let us continue with this analysis little further to see what kind of behavior we can we can expect for a 2 by 2 system. Now, what roots this this equation will have will be see; we are interested is only real part of lambda. So, for example if the second quantity T square by 4 minus D is 0; if it is 0, then whether the Eigen value is negative or otherwise will be determined by simply the sign of this T. On the other hand, if it is positive that is T square minus 4 minus D is positive, then we will have to worry about whether this can possibly give you a negative or positive Eigen value. So, it all depends upon how this T square minus 4 by D behaves. So, let us look at what behavior can we expect.

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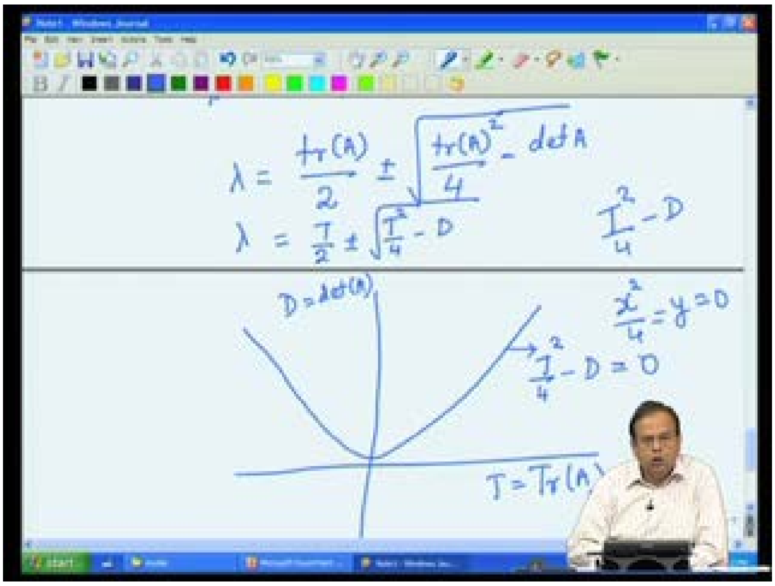

By plotting trace A that is T on the x axis and determinant D on the y axis. So, if I look at, if I write T as x and D as y, what is this equation? T square minus 4 by minus D. It is nothing but x square by 4 minus y equal to 0. What is this equation? This is actually a parabola. We are familiar with this equation. We may be familiar in the form y square equal to A x or something like that. But it is it is a it is a same story; if you say x square equal to y; I mean, that is a that is a parabola. The only difference is we have a parabola, which looks something like this. So, this parabola is T square minus 4 minus D equal to equal to 0. So, now let us look at what happens to my Eigen values depending on the values of my T and D? Now, in this in this particular particular region; so let us let us try to look at that value in more detail.

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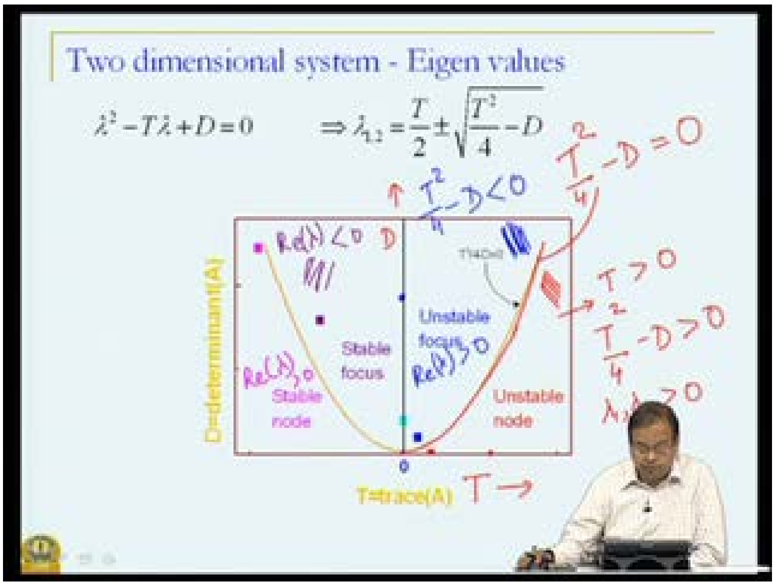

So, what we are seeing here is the same thing; trace T versus determinant determinant D on the y axis with 0 0 being here and this is T square by 4 minus D equal to 0. Now, as we see here, this parabola divides this divides this phase plane in to several regions and let us examine those regions one by one by one. Let us first look at this region which is below this side in the positive quadrant. Now, what is a characteristic of this region? Here, we see that trace is T is positive. We are on the positive side and what about T square minus T square by 4 minus minus D? What do we what can we say about that? Now, how do we determine that? You take any point for example here.

If my D is 0, then I know my T square by 4 minus D is positive and that must be the case for all the points which are below these; that is this shaded region. So, what is happening here? My T square by 4 minus D is also greater than greater than greater than 0. If that is the case, if that is the case then what happens to my Eigen values? If my T square by 4 minus D is also greater than 0; T is T is greater than 0, D is D is obviously positive. We are looking at only positive number. We know that my Eigen value is positive. As a positive, they are first of all real; because square root of a positive term is a real number. And this is T by 2 plus some positive quantity, where T itself is also positive; that means one of the Eigen value is definitely definitely positive.

And the other one will be also positive; because we know that T square by 4 square root minus D will be smaller than T by 2. So, both Eigen values will be will be positive. So, here we will have lambda 1, lambda 2 real and positive; that is for this particular

particular region. Now, what about this another second region? That is that is shown over here; that is above this curve. So, I am now going to use this blue line above this curve; but in the positive positive quadrant. What is happening to what is happening to T square by 4 minus D in this region? This must be less than 0; because it is above this point and easy to check that, take T value to be 0 any point on this axis. What will happen? Any point on this axis, T is 0; D is positive.

So, we have we have a value which is less than 0 right. If this is less than 0; that means, square root of that is a complex number, so the Eigen value real part will be determined simply by the magnitude of T and what is happening to the magnitude of T here; that is positive or the sign of T? What is happening to the sign? So, we have here once again Eigen values are complex; but real part is positive for both the Eigen values right. So, once again real part of lambda is greater than 0 here. By our definition of stability of a steady state, if I have real part greater than 0, then the steady state is stable. So, both these blue region and red region, the steady state is unstable. What happens if you come to this region? What is happening here?

Here by the same argument, we can we can show that first of all T square minus 4 T square by 4 minus D is less than 0; T is negative. So, the real part of lambda is less than 0 in this quadrant and similarly, here also T is negative. This is this is greater than greater than 0. By the same logic, here also real part is greater than greater than 0. So, we have stable node, stable stable focus. Now, what is this business of node and focus? So, essentially what we are saying is on this part let me recap. So, what did we say? We had a two-dimensional problem for which, we had a steady state. We had its Eigen values and depending on the value of trace and determinant, whether it lies in this region or this region or this region or this anyone of these 4 regions. We have different types of stability. We will see a example.

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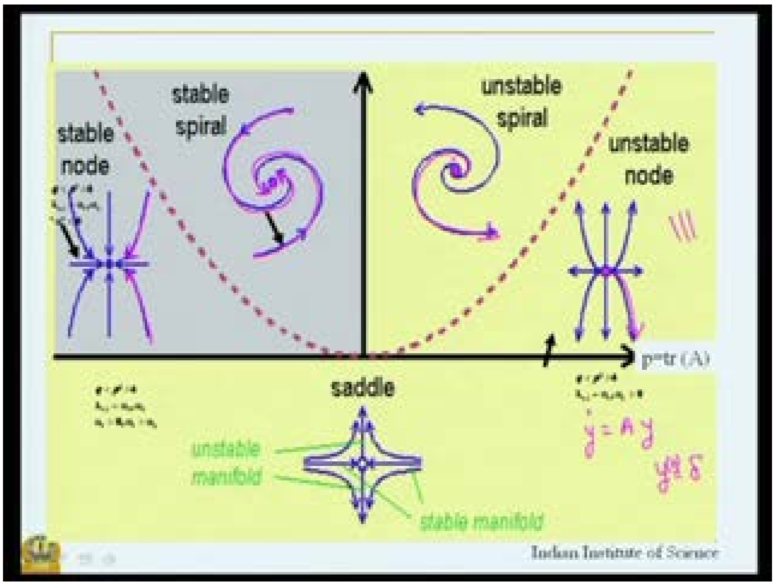

But before we do that, what is this trace node and and business and and so on? So, here is the extended version. So, now what happens is this node or spiral or focus these definitions are given or nomenclature is given, based on how will be the response of the system to the perturbations. So, what is you remember, we are looking at y dot equal to A y. So, if I give some perturbation y of 0 as delta, how that how that behavior will look like? Just in the previous slide, we saw that this was this was an unstable region. So, here the response of the system is to go away from the... So, steady state is my 0. So, this is how the response looks like?

It is called stable unstable node. For this as a steady state, if I give small perturbation, the response is spiral in nature. It is unstable; it is going away; that is my perturbation is getting magnified. It is going away from the from the steady state and therefore, it is unstable spiral. For this particular region, this is the steady state. My response is a stable spiral. It is a stable steady state asymptotically stable. So, any perturbation actually tends to die down and we get to the original steady state; but in a spiral manner. And this region is where, real part of alpha is less than 0; we have we have stable stable node; we have ofcourse saddle point as well.

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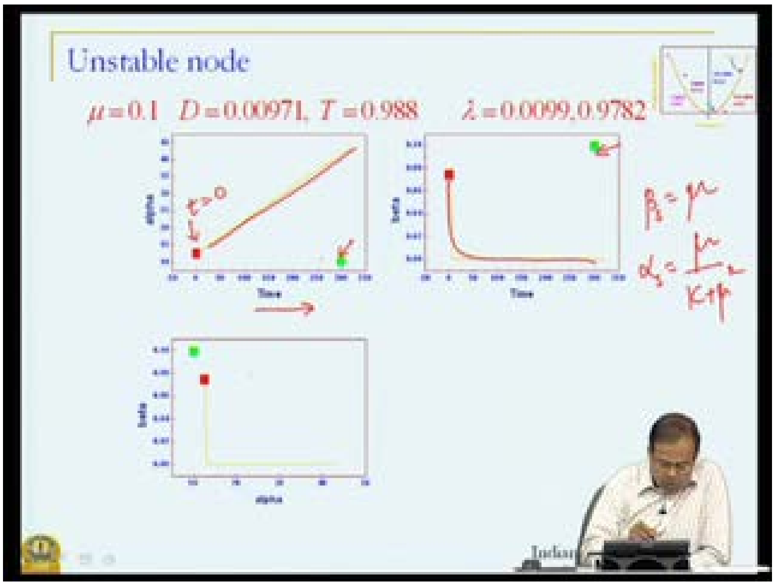

So, let us take an example. So, let me let me let me just recall let me just recall that what we had got was this is our steady state solution. This is my steady state; steady state Jacobian evaluated at steady state. So, we see that it all depends on this value of parameter mu. So, if you fix the value of kappa, what steady state I get will be determined by this mu and which in turn will determine my Jacobian matrix and the trace and determinant and therefore, the Eigen values. So, what we are seeing here and in the previous example; this is what this is what we are we are actually actually seeing.

That depending on the values of mu, I will have steady state solutions in different regions; for example, this blue point or red point or green point violet point and so on maroon point and so on. So, let us look at one example. If mu is mu is 0.1, then substituting all those values; I get my determinant and my trace and my Eigen values, which is trace by 2 plus or minus square root of trace by trace square by 4 minus determinant. And I get my my steady state steady state which is which is unstable. Now, how do I what do I what do I make out of this? So, this is the point which is actually in this this particular particular region.

As the as the name suggest, it is it is over here. So, this is my this is my actually steady state steady state solution of alpha and alpha and beta; that is this green point is my steady state value. You can see beta is 0.1; because solution is… What was our solution? Our solution was beta s is equal to mu and alpha s is mu by kappa plus mu square. So, that is that is some solution. So, for a value of mu equal to 0.1, this is my this is my solution. But if I start with steady state or small perturbation from that; so this is my starting point at T equal to 0 and based on the analysis that we saw, namely we have our our solution in this region which shows unstable node.

So, what happens essentially is as time progresses as time progresses instead of going towards the steady state, we are actually moving away from the steady states. So, this is my trajectory. We are actually moving away from the steady state and that is what is meant by unstable unstable node. So, we do not we do not go towards the steady state; but we rather we move away from the away from the steady state. Now, let us let us look at the behavior of alpha and beta in the phase plane and this is how, the behavior looks like. We are actually moving away from the steady state.

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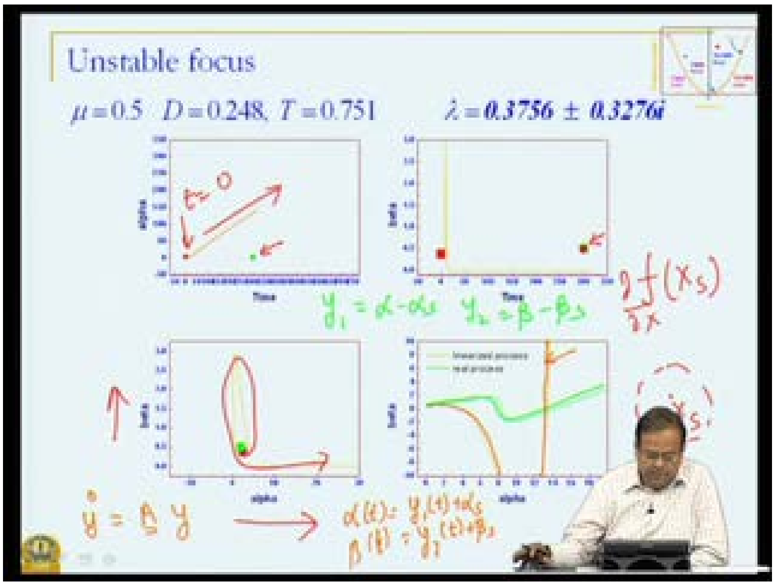

What if what if steady state is unstable focused? That means, our solution or our steady state trace and determinant are in this region; that is in this region, blue region. So, for a value of mu equal to 0.5, for value of mu equal to equal to 0.5 we have actually real complex Eigen value Eigen values and real part of which is positive. So, once again unstable steady state; but behavior is now like a focus. So, this is my this green point is my again the same plot alpha and beta versus time. So, this is supposed to be my steady state. So, if I were to start if I were to start at T equal to 0, at this point once again instead of going to the going to the steady state, I actually go away from here.

Seen in this phase plane of beta versus alpha, green is my steady state; red point is my starting and we see a spiral behavior. We are going completely away from it. But this also brings us to another idea which actually I want to show it with this particular figure.

Remember while determining this stability, we have considered linearized version of the process. So, linearized version always implies that our assumption of linear linearization is always realistic and hopefully applicable, only if the perturbation is very small. Or in other words, when we linearize a function around a point x s, when we linearize it, let us say we say del f del x and so on.

This linearization is valid. Suppose this is my point x s, then this linearization is valid only in the small neighborhood of x s. What it implies is this idea of stability is strictly applicable only if, we are considering small perturbation from the steady state. We can only confidently comment on the behavior for small perturbations. If perturbation is large, we never know what kind of solution solutions we will get and this is actually illustrated in the next plot. See here, what I what I what I have shown is two different different behavior. See for that perturbation, I can generate the response of alpha versus time and beta versus time in two different manners.

One is solving an alpha dot and beta dot equation; that is my mass balance equations directly and this is how, that direct integration solution will will look like. So, those mass balances whatever we had in the dimensionless form, we integrate them integrate them directly. Now, other way of generating this solution is remember we had made perturbation variable. So, let us say y 1 is alpha minus alpha s and y 2 is beta minus beta s right. So, now I can generate the linearized version of solution by solving y dot equation equal to A y. We know the solution of this; where A is the Jacobian matrix.

So, get y 1 of t and then say alpha of t is y 1 of t plus alpha s and beta of t is y 2 of t plus beta s. If I do that, if I do that then my alpha beta behavior is actually something like this; which is completely different than the behavior of the actual system. So, what I call? This is the behavior of the linearized system; whereas, the green line is the behavior of the real system and you can see for yourself the difference in the in the behavior. So, the point I am trying to make is that this idea of linearization is possible or is applicable only for small perturbations. If you have large perturbation, we cannot use this idea.

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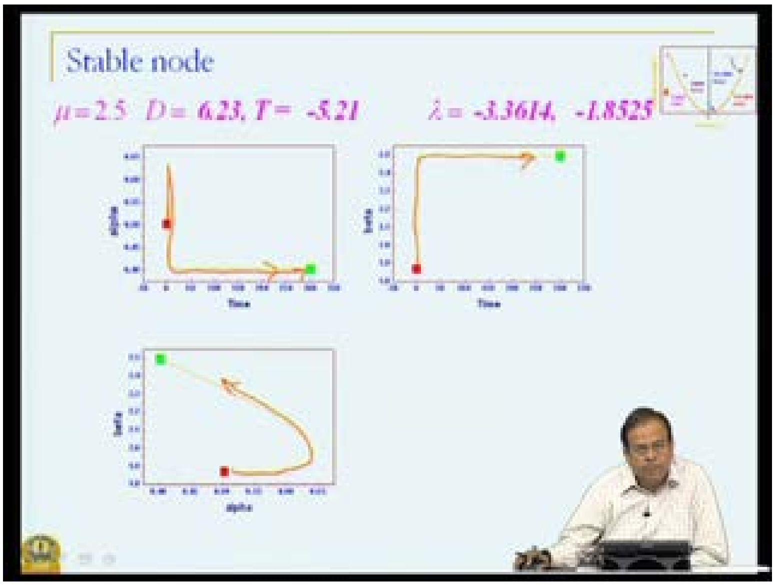

Moving along with different values of alpha and beta; so suppose we take alpha and beta, a mu value to be 2.5; that is we are in this region of stable stable node. Then, what we find is both Eigen values are real and negative and the solution is stable node. So, we start this is green point once again is our is our steady state solution. We start from perturbed value, which is shown by red point and what we see here is actually we first seem to deviate; but we come back to the steady state. This same thing for same thing for beta and then this is the behavior in terms of alpha beta phase plane behavior.

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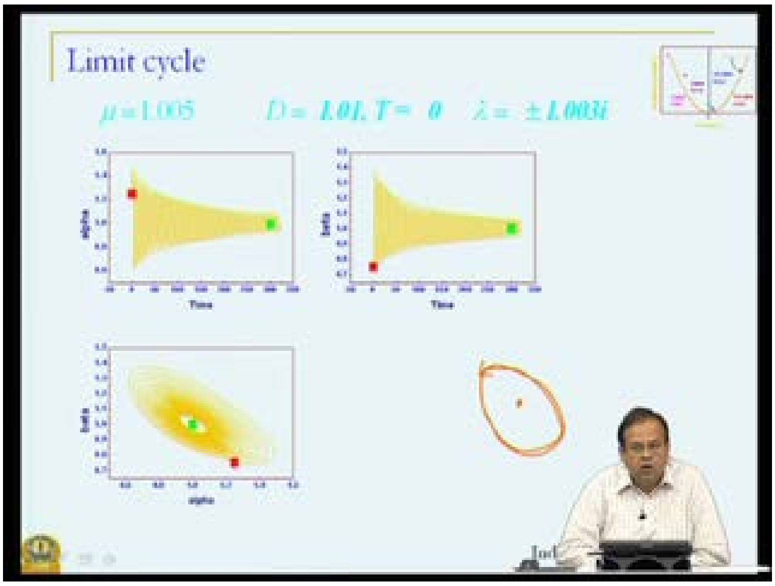

Now, comes an interesting situation, where my mu is 1.005. So, actually we are if you look at look at our solution over here. If my mu is 1.005, then it turns out that my trace is 0 and I am at this particular point. Now, if trace is 0, then what is the Eigen value? The real part is 0 and we have complex Eigen values with plus or minus I and the behavior is what we get is a limit cycle or which is shown here. So, this is my steady state, green point; red point is my starting point. And now, we see an oscillatory behavior such that even if you wait for a long time, the behavior never or the solution never converges to this new steady state. But it circles around that; infact, seen clearly in this phase plane behavior. So, this is my expected steady state value. But I am always ending up in a limit cycle. So, this is where the real part of the Eigen value is 0.

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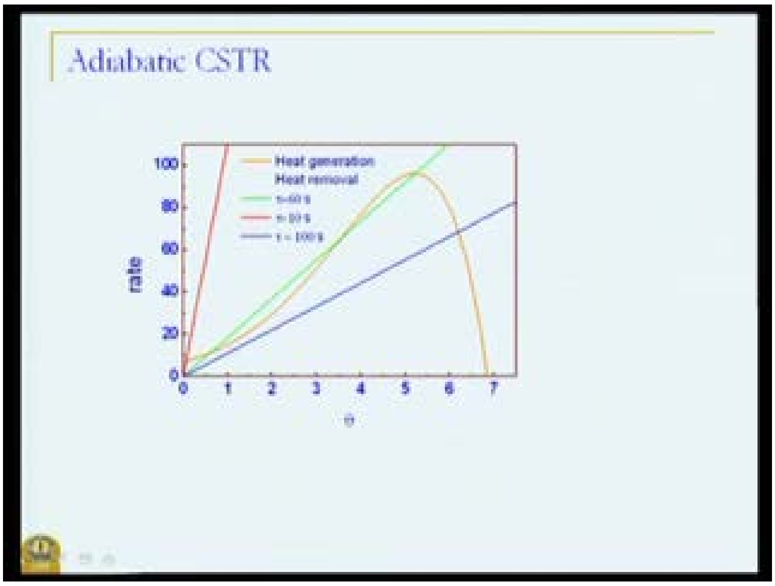

So, this in short is the is the summary of or an example of how we use steady state analysis. Let me let me quickly go through the same similar similar analysis. Let us say for our reactor, which we saw in the in the last session; that is non-isothermal reactor.

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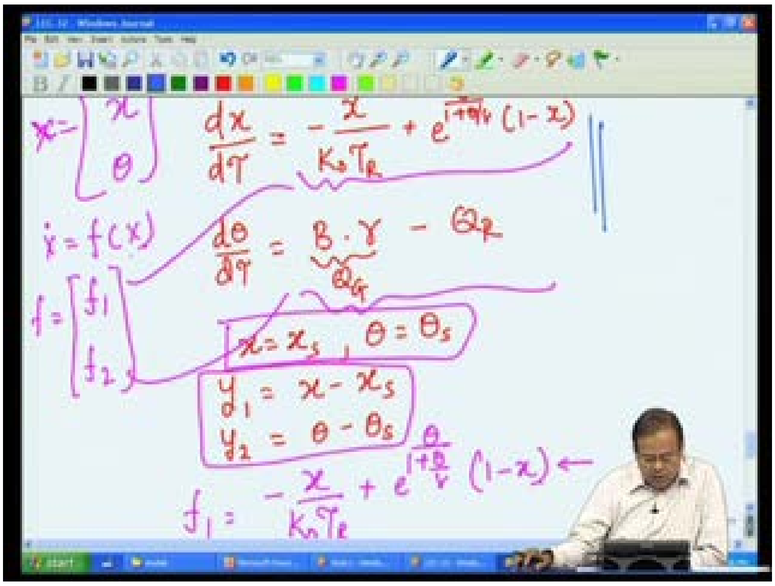

So, if I can get this; So, this was our example; we went through this example last time; that is our non-isothermal CSTR and these are our x; that is vector x, which is dimensionless concentration x and theta our dynamics which we define as f 1 and f 2, where my f 1 and f 2 are this particular particular matrix.

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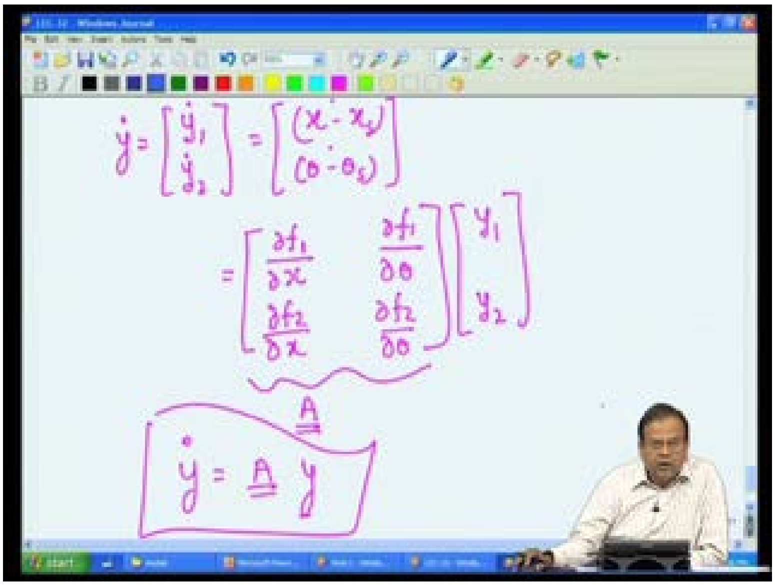

And then, we have we have this del f 1 del x del f 2 del theta and so on. So, now if I write my stoichiometric matrix using all this all these quantities f 1, f 2 and so on.

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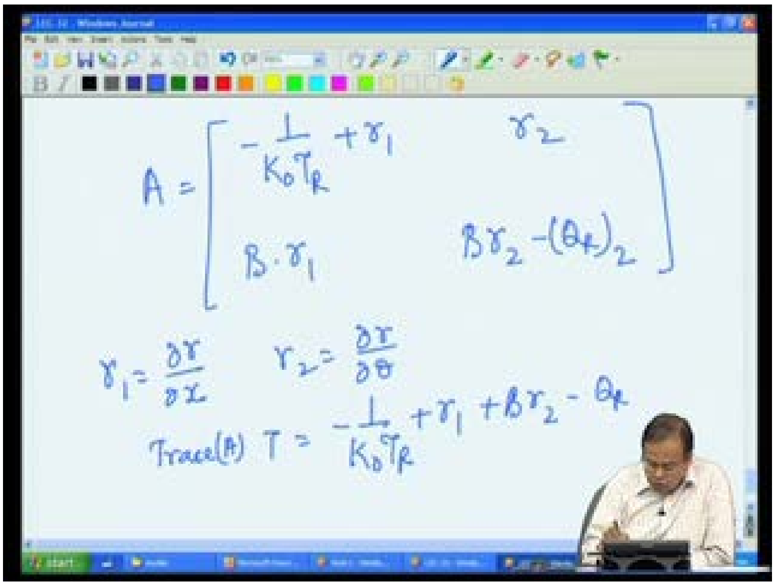

I will get my Jacobian matrix as 1 over K naught tau R plus r 1 r 2. I will just come to what is r 1 and r 2? This r 1 is nothing but del r del x and r 2 is nothing but del r del theta; remember r is our reaction rate. So, this is my this is my notation. So, I have this this particular particular matrix. So, again what is the what is the trace A? That is T for this is nothing but addition of addition of these two quantities. So, which is 1 minus K naught tau R plus r 1 plus B r 2 minus Q R 2 and I will have I will have determinant.

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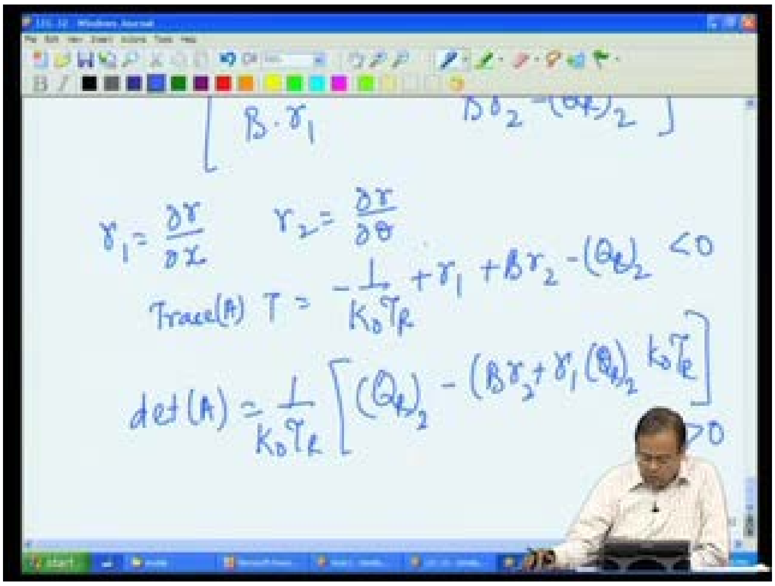

Determinant of A which I can write by doing some simplifications as 1 over K naught tau R in to Q R 2 minus B r 2 plus r 1 Q R 2 K naught tau R and if you recall what should be our condition for stability? Our trace should be negative and our determinant should be positive; that ensures that my my steady state is stable. So, now if we if we use the steady state information that is the steady state, when when this quantity is f 1 and f 2 are 0 and if I if I use all that, then it turns out that this particular condition.

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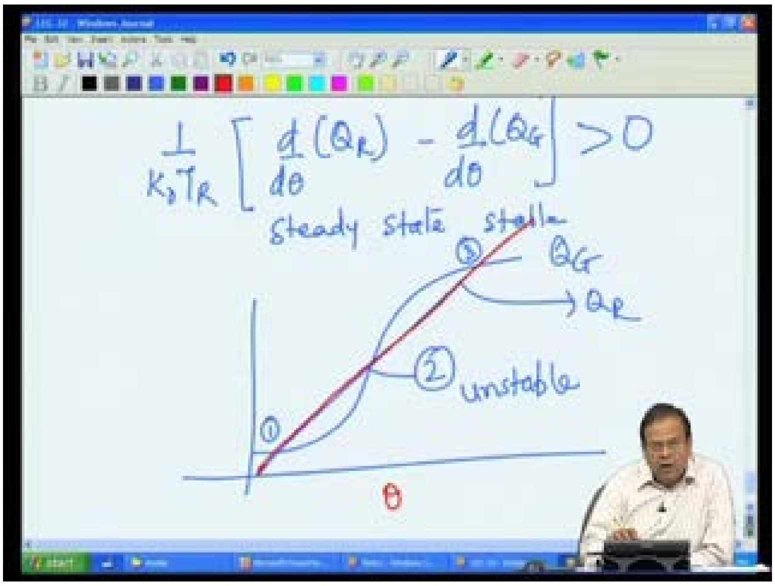

This particular condition reduces to 1 over K naught tau R into d d theta of Q R minus d d theta of Q G should be greater than 0. If this condition is satisfied, then my steady state is stable. You will recall that this was exactly what we saw in a in a graphical sense, when while looking at looking at the behavior of unstable and stable steady state. We said we said that let me let me let me just redraw these figures. What we said was this was our Q G curve; this was our Q R curve and we said at point 1 and 3 are stable; this is unstable. Let me let me draw Q G Q R curve by red line. So, what is the condition for stability? We said that the slope of the heat removal curve with respect to temperature.

What is this? This is again theta with respect to temperature should be higher than the slope of heat generation curve which is precisely what is happening at point 1 and 3; whereas, this condition is violated at point 2. Slope of this blue line is higher than the slope of the red line and therefore, we find that this steady state is unstable. So, with this, we will conclude our discussion on unstable or stability of the steady state. Just to recap, what we saw was we have a dynamic system and we have a steady state solution for this dynamic system. We are interested to find out whether the system is stable or unstable.

And we do this by doing a linearized analysis, considering the Jacobian which is the partial of the f with respect to x or partial of the dynamics with respect to x and looking at the Eigen values of this Jacobian. If the Eigen values have real negative part, we say that this system is stable. If the real part is positive for any atleast one of them, then we have an unstable steady state. What is the meaning of stable steady state? In a simple word, a stable steady state is a one where if we introduce perturbation to this stable steady state. These perturbations die down as time progresses; whereas, unstable steady state is a one where perturbations simply expand. Practically, it implies that without any control system, we will never be able to reach unstable steady state; whereas, same is possible for a stable steady state. Thank you.