Advanced Mathematical Techniques in Chemical Engineering

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Lecture No. # 13
Stability Analysis

Very good morning to everyone. So, we were looking into the applications of Eigenvalues and Eigenvectors in various chemical engineering problems. So, in the last few classes we have looked into the solution of ODE, solution of the set of algebraic equations, set of ordinary differential equations and homogenous and non-homogenous equations, those will be arising out of the chemical engineering processes and how Eigenvalues and Eigenvector method can be applied quite elegantly and replacing the numerical techniques. And, including, involving, even if you go for a higher dimensional operation the numerically calculated values will be done quite easily involving very small subroutine of elementary in nature.

Now, what we have seen in the earlier classes is that we have developed the theory based on this, to solve the set of algebraic equations and ordinary differential equations, both homogenous form and non-homogenous form, and along with that we have given we have discussed some of the problems how to apply the Eigenvalue Eigenvector method for their solution.

Now, in today's class, we will look into another application of Eigenvalues and Eigenvectors that will be appearing in the continuous domain. So, we will be looking into the Stability Analysis of any chemical engineering processes this stability is very important, as far as the chemical reaction engineering and chemical engineering processes are concerned, because consider any chemical reactor, if it is operating under the stable operating conditions then you can ensure the quality of the product we are going to get.

So, if the quality of the product is ensured, then it is marketability and market value will be ensured; so, we can do a very good business. If the stability of the system is not appropriate, then one cannot be very sure about the product quality; so, Stability

Analysis is very important, so we will be basically looking into the various theorems that will be applicable for analyzing the stability of any chemical engineering processes and after that we will be doing the analysis based on this theory and trying to extract the features or the set of operating conditions, under which the operation can be carried out under stable conditions.

So, stability is very important as far as the chemical engineering processes and whatever we will be doing from today's class onwards, that will be extremely important for the chemical engineers to analyze the stability of a system.

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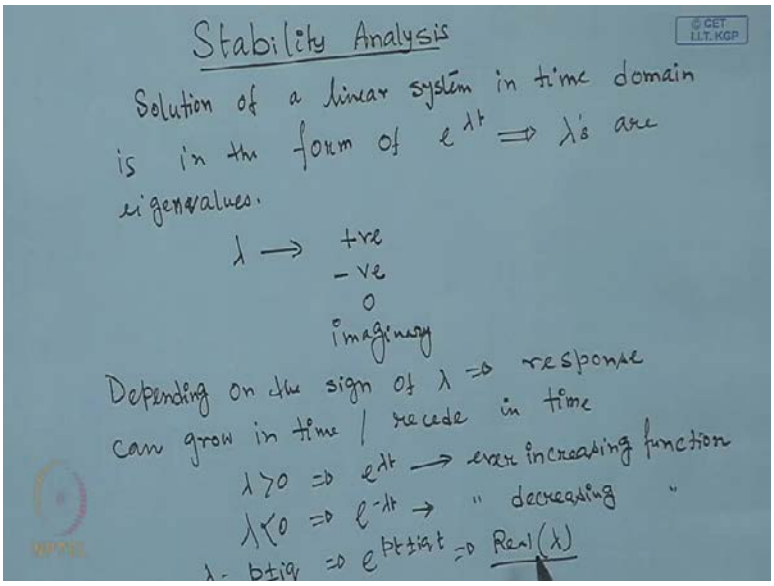

So, let us look into the various methods involving Eigenvalues and Eigenvectors and we will develop the theory for a Stability Analysis. Now, if you look into the solution, that we have talking about that the solution in, of a system, of a linear system, even it is a valid for the non-linear system as well, solution of a linear system will be in time domain is in the form of e to the power lambda t, where typically the lambda's are Eigenvalues of the relevant problem. Now, this lambda become, this lambda can be positive, it can be negative, it can be when 0, it can be imaginary; if it is imaginary, then of course, it is a counter, the conjugative will be appearing; so, if there are two roots then there is a possibility of having imaginary roots.

Now, there is, if you can see in this problem - that if the depending on the sign of lambda, the response can grow in time or recede in time; that means, if lambda is positive then e to the power lambda t is ever increasing function. On the other hand, if lambda is never negative, then e to the power minus lambda t is ever decreasing function. If lambda is imaginary, let say p plus minus i q, then e to the power, this will be entirely depending upon the real part of the lambda.

Now, if real part of lambda is greater than the 0, then the response will grow in time; if real part of lambda is negative the response will die down in time; so, if e to the power lambda is positive ,if it is e to the power lambda t ever increasing function; that means, if you put a disturbance in a system, it will grow in time monotonically; on the other hand if we put a disturbance in a system for lambda is negative the response will die down in time.

So, therefore in case of imaginary roots, it entirely depends on the real part of the root; if root is positive, then lambda then the disturbance will grow in time; if this real part is negative, then the disturbance will die down or decay in time. Now, these will be extremely important as for as the stability of the system is concerned, that if you impart a disturbance in the system, if the response grow in time then we are looking, we are basically landing up into a system, which is not stable. On the other hand, if the response decays with time then will be landing up in a system, where, which will be stable.

So, the aim will be to have a stable region, so there will be conditions that this Eigenvalue will be negative then will be getting into the stable region and of course that will happen under a certain combination of the parameters, where the parameters are basically combination of operating variables. So, under those operating variables, so that they will satisfy those conditions, the system will be operating under stable steady state.

Now, in order to develop the theory, we will just take up a chemical engineering application and will take up whatever we have done earlier that, is a, in case of contraction mapping will take up an example of continuous start tank reactor, which was non-isothermal. So, we take up those conditions of the energy balance, those equations of energy balance and mass balance, to start up with our discussion in the context of stability of chemical engineering processes.

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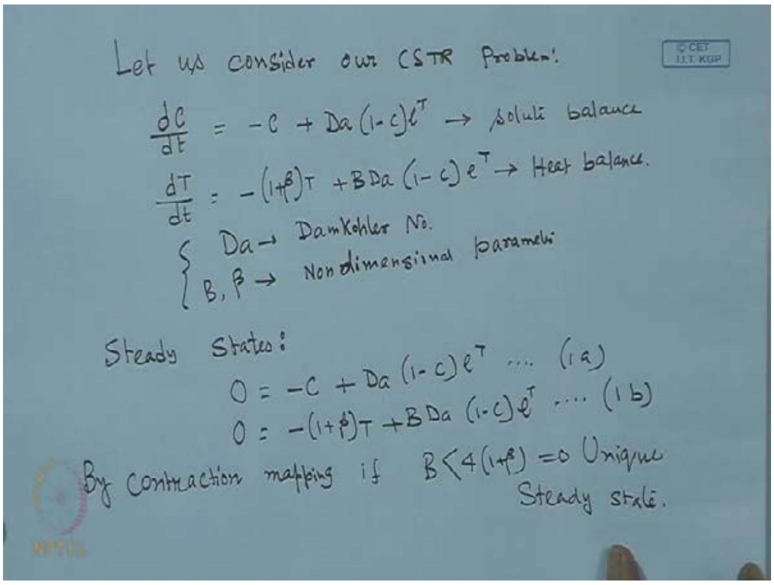

Now, let us consider the CSTR problem, whatever we have developed discussed in case of contraction mapping, our CSTR problem. We have the solute mass balance was given by d c d t is equal to minus C plus D a 1 minus C e to the power T; this is nothing but solute balance. And d T d t is be given by minus 1 plus beta T plus B times D a 1 minus C e to the power T; so, this will be the heat balance equation. The parameters in a system are Damkohler number, beta is a non-dimensional parameter and B is another non-dimensional parameter; now, these three are the parameters of the system.

Now, let us look into the steady state of these system; the steady states will occur when this time derivate will be equal, to put, will be force to equal to 0; so, the steady state will be occurring by putting 0 is minus C plus D a 1 minus C e to the power T; this is equation 1 a. And minus 1 plus beta T plus B D a 1 minus C e to the power T; so, this is equation 1 b.

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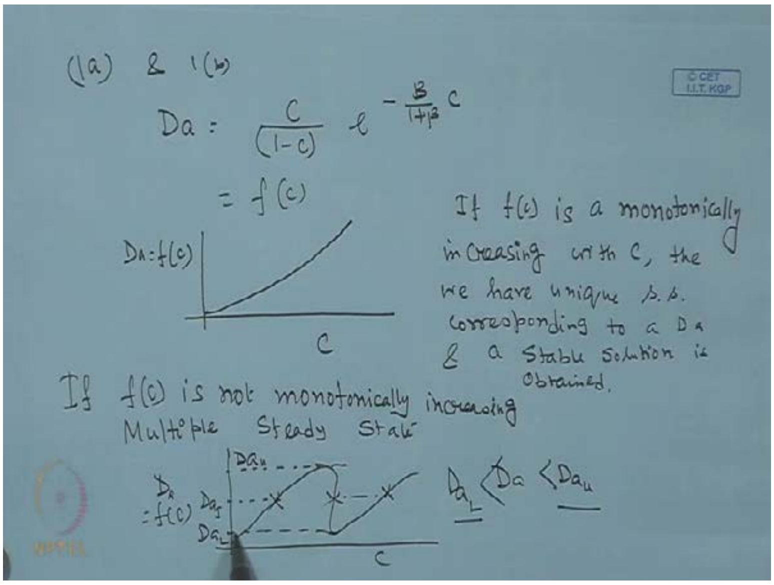

So, we have already seen that by contraction mapping, if B is less than 4 into 1 plus beta, then we will be having unique steady state for this particular problem. So, we have already seen by contraction mapping that if B is less than 4 into 1 plus beta, unique steady state exists. So, we can combine equation 1 a and 1 b and we can write D a is equal to C 1 minus C e to the power minus B divided by 1 plus beta times c.

So, this will be a function of concentration only. So, if we plot D a or f of C as a function of C, we can see that it will be an ever increasing function; now, if this is the case then if we have f C is a monotonically increasing function which increasing with C. Then we have unique steady state corresponding to a D a to a Damkohler number and a stable solution is obtained; this we have proved earlier during the discussion of contraction mapping that if f C is monotonically increasing function with concentration, then for that, for those particular D a Damkohler number will be getting the stable steady state.

On the other hand, if f C is not monotonically increasing then will be landing up with multiple steady state; it means, if f of C is not monotonically increasing then we may land up with multiple solution or multiple steady state; convince, if we plot D a f of C D a is same as f of C verses concentration if the plot looks something like this, it is not monotonically increasing function, it is decreasing and then again it is increasing; then you will be having, they, a particular D a may be here intermediate, where there will be a solution here, there will be a solution there, there will be a solution there; so, there will be three solutions they may exits.

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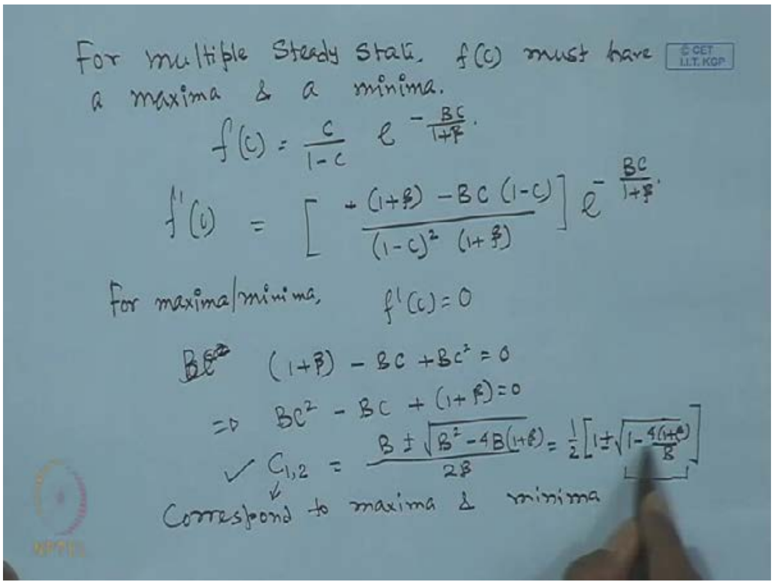

So, you can have the upper limit, so if this is the case, then you will be having the upper Damkohler number D a u and this you will be getting a lower Damkohler number D a L; so, there will be Damkohler number in between D a L and D a upper, for which one can have a more than one solution or more than one steady state. So, between this limit D a l and D a u, one can have multiple steady state of this particular problem. So, of course, what we can understand from this discussion is that in order to have existence of multiple steady state, the f C will be having a maxima and will be having a minima, then only if the function of concentration will be having a maxima and minima, then only one can expect of occurrence of multiple steady state. Now, let us put this condition in this particular case; so, for multiple steady state f C must have a maxima and a minima; so, f of C should be equal to C divided by 1 minus C e to the power minus B C divided by 1 plus beta, so for in order to have maxima or minima.

Let us get a differentiation of this, so this becomes minus, this becomes 1 plus beta minus B C into 1 minus C divided by 1 minus C square into 1 plus beta e to the power minus B C divided 1 plus beta; so, this is the differentiation of f of C. So, I am just writing the final expression, so for maxima or minima f prime C will be equal to 0.

So, therefore one can get this equation B C square, so if basically the numerator will be equal to 0, so it will be, 1 plus beta minus B C plus B C square is equal to 0; so, you will be having condition B C square minus B C plus 1 plus beta is equal to 0. Now, this will be having two roots, this is a quadratic in C, so it will be having two roots. So, let us find out what this two roots are, they will be minus B, so it will be plus under root B square minus 4 a C ,so B times 1 plus beta divided by 2 a, that means, 2 b.

So, if we take B common from here, so what will be getting is that 1 by 2 1 plus minus under root 1 minus 4 into 1 plus beta divided by B; so that is the condition, there are two roots, one root corresponds to maxima and other root corresponds to minima; so, these two roots corresponds to maxima and one for minima. Now, we can have, in order to have a real solution, we can have the condition on this part, that this 1 minus this part should be greater than 0 in order to have a real root or real solution.

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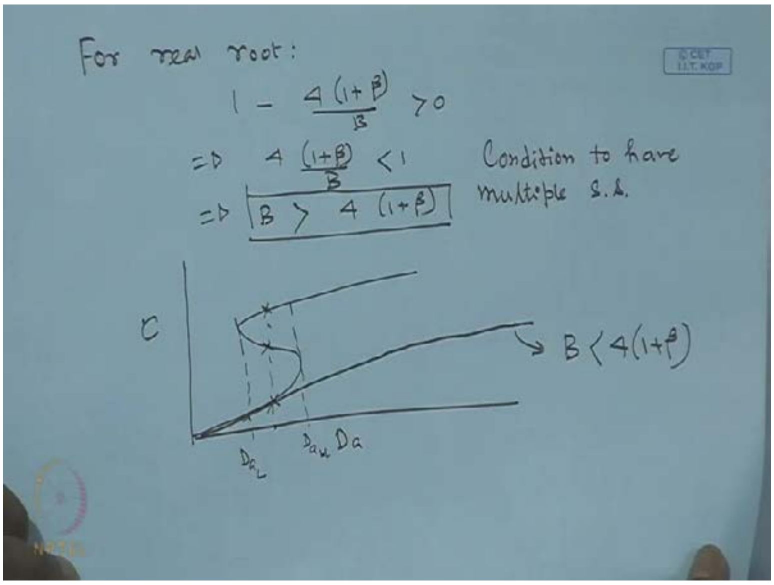

So, let us do that for real root the quantity within the under root sign will be must be greater than 0; so, therefore 1 minus 4 into 1 plus beta divided by B should be greater than 0; so, therefore 4 into 1 plus beta divided by B should be less than 1; so, will be having B is greater than 4 into 1 plus beta. So, this is the condition for this particular problem in order to have a multiple steady state.

So, this becomes that condition to have multiple steady state of this problem, this is just a counter part of whatever we have obtain for the condition, of unique, having the unique steady state of this problem. So, if you remember that the condition, we obtain from contraction mapping for existence of unique steady state is B less than 4 into 1 plus beta solve; obviously when B is greater than 4 into 1 plus beta that is a condition for the multiple steady state and we have derived that.

So, now, if you plot C verses Damkohler number verses C or C verses Damkohler number whatever way, so this will be, they, there may be one response like this, there may be a response like this. So, this is, in this case for every C will be having only for every Damkohler number, you will be having only one C, for every, for this curve, in the, for the lower curve for every existence of Damkohler number, you will be getting only one concentration, one solution steady state solution. And therefore, on this curve the unique steady state exists, so B is less than 4 into 1 plus beta.

On the other hand, if you talk about this range of Damkohler number, for this Damkohler number any Damkohler number between D a upper and D a lower; it there will be having three steady state or multiple steady state existing for this problem. Any Damkohler number beyond D a u will be leading to a steady state on the upper branch; any Damkohler number below the value of D a L, one will be getting a solution at the lower branch; for any Damkohler number laying in between D a u and D a L, it will be having a multiple steady state in the system.

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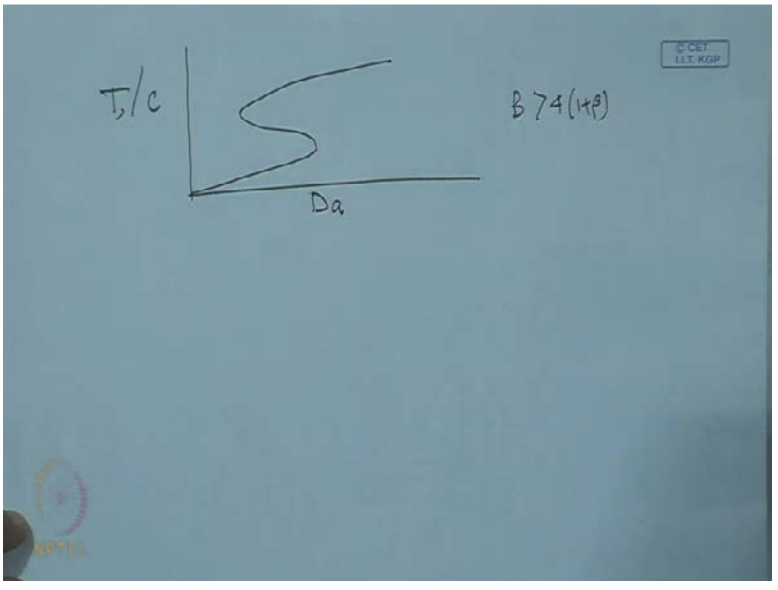

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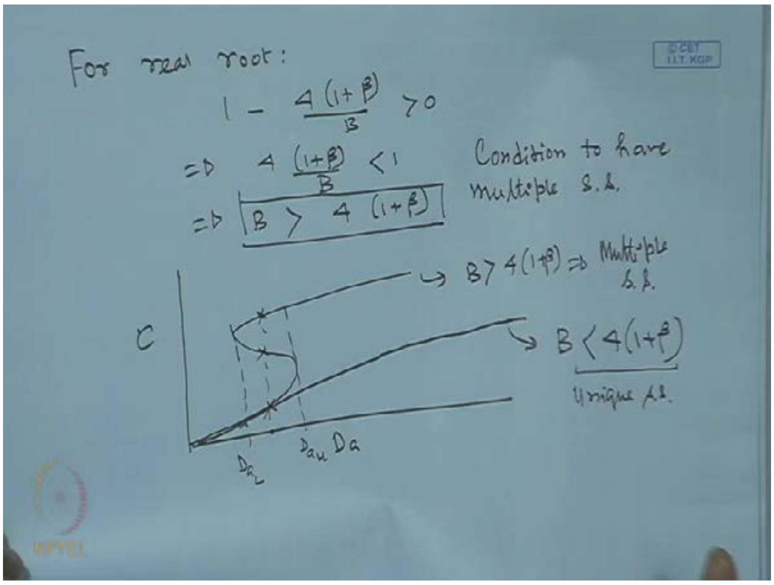

So, if we plot now for this particular problem, if we plot now, T or C verses Damkohler number for multiple steady state part, will be getting a curve like this; this is the condition for B greater than 4 into 1 plus beta. So, if we summarize whatever we have obtained in the earlier slide, that this is for this case B is greater than 4 into 1 plus beta; that means, this is for condition for unique steady state and this is the condition for multiple steady state.

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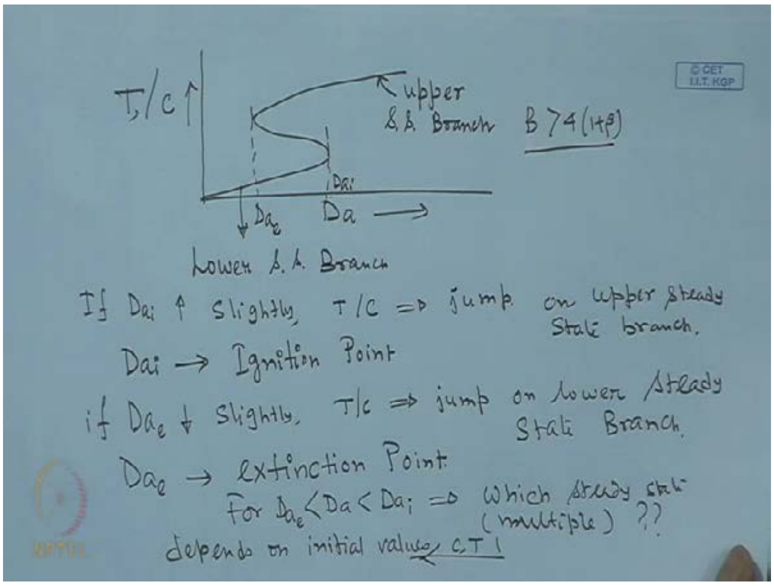

So, next, we have the T and C verses Damkohler number, for the condition B greater than 4 into 1 plus beta. This is known as upper steady state branch, and this is the lower steady state branch. Now, suppose, this is D a i, so if D a i increases slightly both T and C, they jump on the upper steady state branch; therefore, D a i is called an ignition point. So, if you just slightly increase it is beyond I, Da I, it will go to the upper steady state branch; so, Da i is called the ignition point.

On the other hand, the other limit is D a e, if we slightly decrease D a e, if D a e is decreased slightly, then T or C, they jump on lower steady state branch; so, D a e is known as extinction point. So, which steady state will be, if a in between, the D a e and D a I, if we operate on any Damkohler number will be having a multiple steady state.

Now, for D a laying in between D a e and D a i which steady state is obtained, that will be entirely depend on the initial values of T and C, which steady state among multiple; that is the question. Then, it entirely depends on initial values of C and T; so, depending on the initial value of C and T, one can get this, the steady state in between. Now, next we talk about all these phenomena can be properly explained, if we talk about a phase plane plot.

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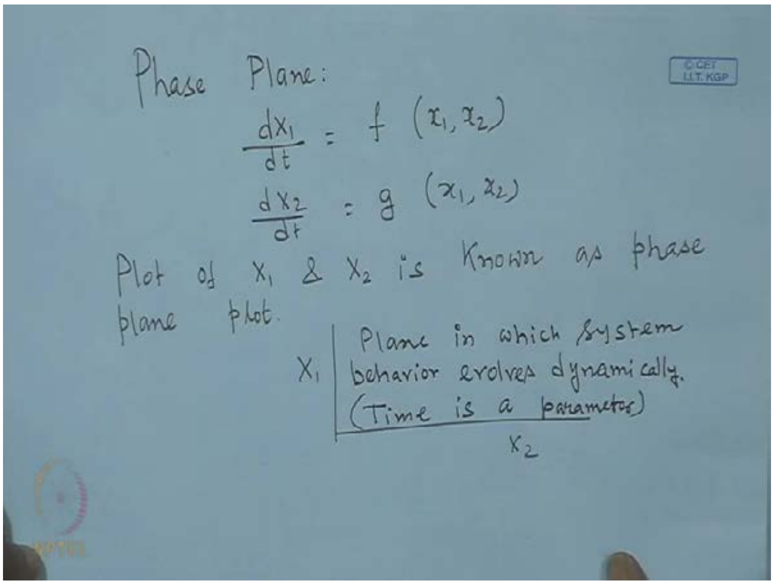

So, let us look into the phase plane plot; so, first let us defined what is a phase plane; suppose, any system is define by two ordinary differential equations like d X 1 d t is function of x 1 and x 2; x 1, x 2 are the state variable; d X 2 dt is equal to g of x 1 and x 2 then the plane where the system behavior evolves dynamically the variation of x 1 and x 2 is called a phase plane plot; plot of X 1 and X 2 is known as phase plane plot.

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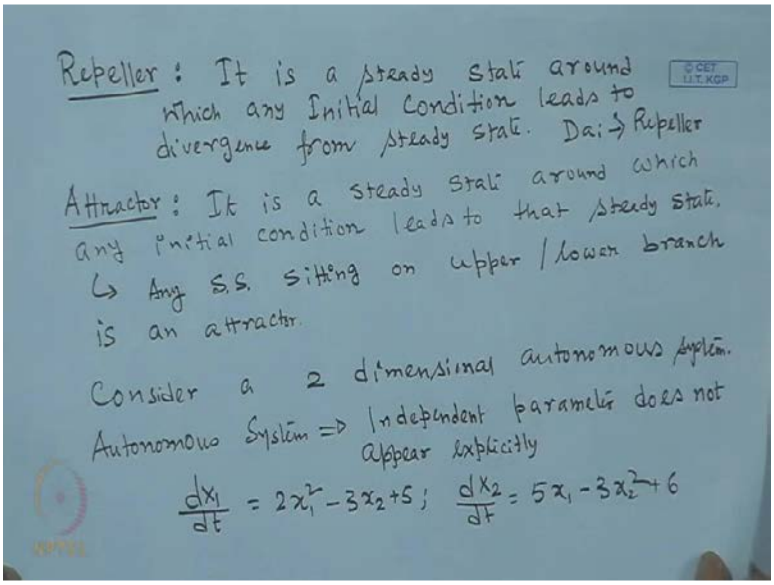

So, if we plot X 1 as a function of X 2, it gives a plane in which system behavior evolves dynamically. Now, in this case, time is a parameter, so that gives the concepts of phase plane plot. Now, let us look into some more concepts and definitions, first one is the repeller; so, let us see what a repeller is, repeller is a steady state, it is a steady state around which, if you have any initial condition that will lead to a divergence from the steady state. So, it is a steady state around which any initial condition leads to divergence from steady state.

So, in the earlier example, D a i is a repeller; so, if we have any steady state about that point, then it will either go to the upper steady state or it will go to a lower steady state. Then attractor, this is a steady state around which any initial condition leads to that steady state; so that steady state is called an attractor.

So, steady state, this attractor may be, the in the earlier example, any steady state sitting on upper branch or lower branch is an attractor. And D a i or D i in the earlier example is a repeller. So, any steady state around D a I, either it will be landing on upper steady state branch or lower steady state branch, on the other hand if any steady state is sitting on the upper or lower branch, beyond the D a i and D a e region that will be acting as an attractor.

Now, let us try to develop the theory of stability for a two-dimensional system, this can be extended for a multi-dimensional system. So, for that, we consider a two-dimensional autonomous system and autonomous system, means, independent parameters do not appear explicitly; if independent parameter does not appear explicitly, then we call that system as autonomous system.

For example, if the said variables are X 1, dependent variables are X 1 and X T and X 1 and X 2 and the independent variable is d t, if it is 2 x square x 1 square minus 3 x 2 plus 5. And if d X 2 d t is equal to 5 x 1 minus 3 x 2 square plus let say 6. Now this system is an autonomous system, because the independent variable t does not appear on the right hand side in either of the equation; so, this is an autonomous system.

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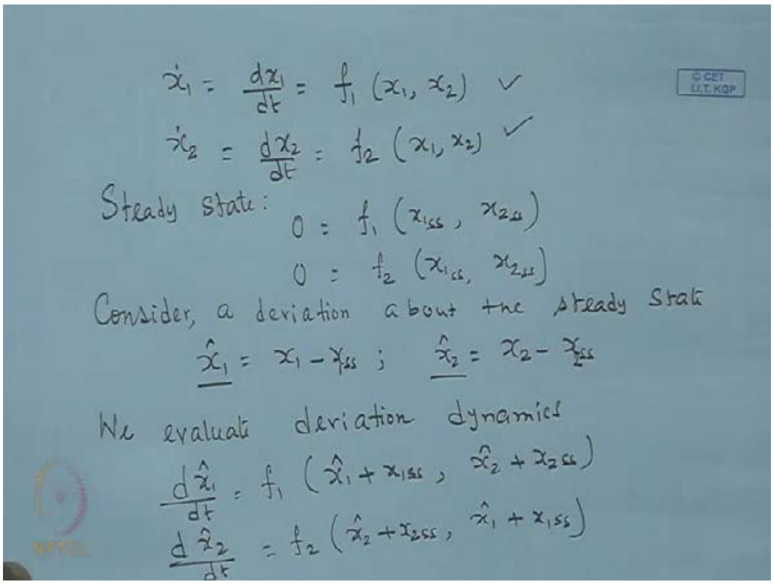

Now, let us consider an autonomous system, where x 1 dot is equal to d x 1 d t and in general this will be a function of x 1 and x 2. And in the second equation, x 2 dot is d x 2 d t is equal to another function of x 1 and x 2; so, it does not the right hand function f 1 and f 2 are inert functions of x 1, x 2 and t explicitly; so that is why they are called autonomous system.

Now, most of the chemical engineering process is they fall under the category of autonomous system. Now, let us look into the steady state solution of this two equation; so, the steady states are 0 f 1 x 1s s, x 2s s; s s stands for the steady state and 0 is equal to f 2 x 1s s and x 2 s s. Now, let us consider a deviation about the steady state and this deviations are x 1 hat is nothing but x 1 minus x s s; and x 2 hat is x 2 minus x s s. Now, in order to evaluate, now what we are going to do, the evaluation the dynamics of the deviation variable.

So, these are called deviation variables of the two parameter, 2 dependent variables x 1 and x 2; this will be x 1 minus x 1 steady state, x 2 minus x 2 steady state. So, we evaluate deviation dynamics, how to evaluate that, we evaluate all the know governing, we write all the governing equations in terms of x 1 hat and x 2 hat. So, therefore d, we can write these two equations as, d x 1 hat d t, in fact, if you differentiate this equation with respect to t d x 1 d t is identical to d x 1 hat d t, so this will be nothing but function f 1 x 1 hat plus x 1s s and x 2 hat plus x 2 s s. And similarly we have d x 2 hat d t is equal to f of 2 x 2 hat plus x 2 s s and x 1 hat plus x 1ss. Now, so, we express all the parameters, the dependent variable x 1 and x 2, in terms of deviation variable x 1 hat and x 2 hat.

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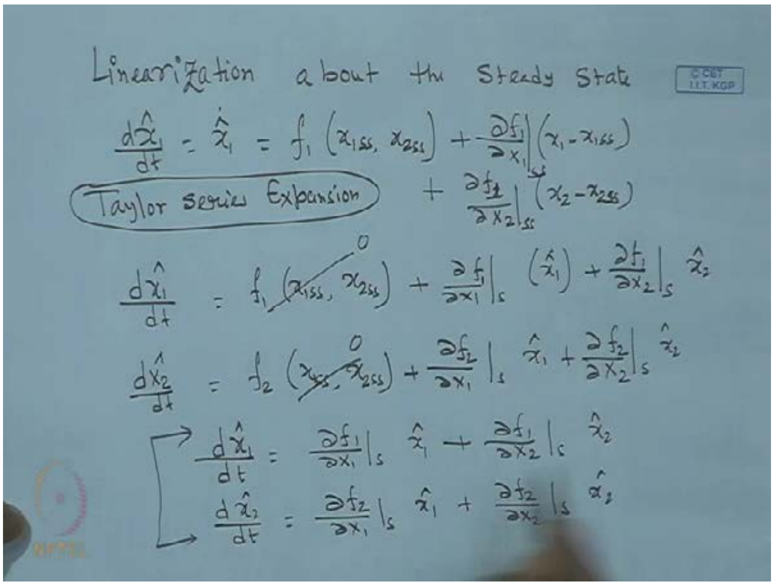

So, next, we linearize the problem about the steady state; next step is linearization about the steady state, if we do a linearization then x 1 d x 1 hat d t or x 1 hat dot becomes f 1 x 1s s and x 2 s s plus del f 1 del x 1 x 1 minus x 1s s plus del f 1 del x 2 x 2 minus x 2 s s. It give a slight deviation about the steady state by test; so we linearize this thing by Taylor series expansion and retain only the first term of the expansion and this derivatives are about the steady state, this vary derivatives about the steady state. So, we retain the first term of Taylor series expansion and delete the higher other terms, because the deviations are extremely small, from the deviations are extremely small compare to the steady state.

So, therefore, we can write d x 1 hat d t will be nothing but f 1 x 1 s s and x 2 s s plus del f 1 del x 1, about the steady state, x 1 hat plus del f 1 del x 2 at the steady state, this will be x 2 hat. So, that will be the governing equation of dx 1 hat the deviation variable the dynamics of deviation variable by using linearization and that linearization will be restricted a to up to the first term and neglecting the higher terms of Taylors series expansion.

Similarly, we will be getting the next part of the deviation variable d x 2 hat d t will be nothing but f 2 x 1 s s x 2 s s plus del f 2 del x 1 and that will be evaluated as steady state, and this will be x 1 hat plus del f 2 del x 2 evaluated at the steady state, and that will be multiplied by the x 2 hat. So, therefore what we can do, we can write these two equation in a compact form and also if we remember that f 1 x 1 s s and x 2 s s were equal to 0 and f 2 both f 1 and f 2 evaluated at steady state, they are equal to 0. If you look into the earlier slide that these were the governing equation of the system, we are considering and at the steady state these will be equal to 0, and f 1 x 1ss x 2ss equal to 0, and f 2 x 1ss x 2ss will be equal to 0.

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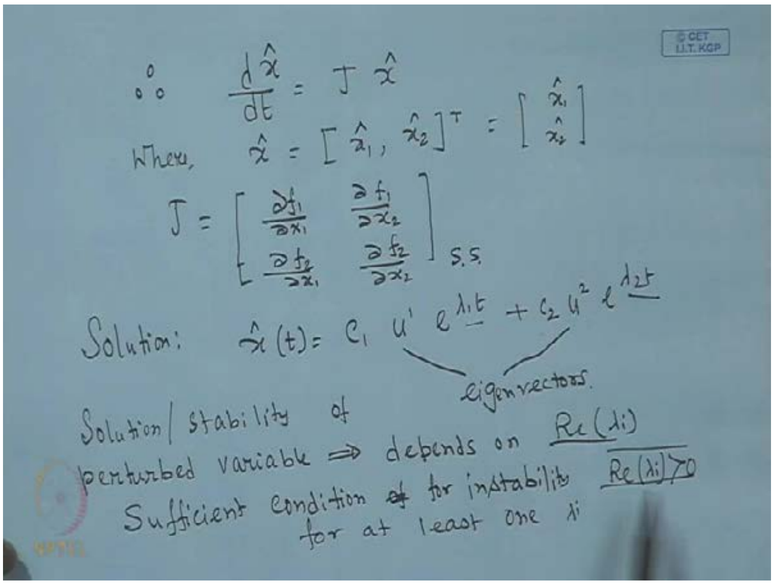

So, therefore, we have every right to make this two equal to 0, so the need at compact form will be d x 1 hat d t in the deviation variables will be del f 1 del x 1 evaluated at steady state x 1 hat plus del f 1 del x 2 evaluated at steady state through a x 2 hat. And d x 2 hat d t will be nothing but del f 2 del x 1 steady state x 1 hat plus del f 2 del x 2 steady state x 2 hat. So, these two equations in the deviation variable can be written in a compact matrix form as, d x hat d t is equal to j times x hat; where x hat is nothing but a matrix, a vector, which will be having two elements x 1 hat and x 2 hat and transpose of that; so, it is nothing but a vector x 1 hat and x 2 hat.

And the Jacobian matrix J becomes the elements of the derivative they will constitute the derivatives will constitute the elements of the Jacobian matrix and these will be del f 1 del x 1 del f 1 del x 2 del f 2 del x 1 and del f 2 del x 2 and all these derivatives which are the elements of the Jacobian matrix, they will be evaluated at the steady state. So, the solution of this equation will be in this form of x hat t will be is equal to c 1 u 1 e to the power lambda 1 t plus c 2 u 2 e to the power lambda 2 t, because it is 2 into 2 matrix, so you will be having a two Eigenvalues lambda 1 and lambda 2 and u 1 and u 2 are high corresponding Eigenvectors. So, stability of the perturbation this terms value variable is nothing but the perturbation variable, through solution of solution or stability of perturbed variable or the perturbation, that we have imposed from outside, they will be entirely depend on sign of a real values of lambda i.

So, real values of eigenvalues will dictate, whether this disturb the perturbation variable will grow in time or it will die down with time. So, if real value of lambda is positive then this disturb, even if one of them is positive, the whole solution the disturbance variable will grow in time; if it is negative then if all of them will be negative, then it will be the stable solution and the disturbed part out variable will die down with respect to time.

So, the sufficient condition for instability is real value of lambda i should be greater than 0. So, for at least one lambda i then, that means, if in a system there are 4 or 5 Eigenvalues, if the real part of 1 Eigenvalue is greater than 0, the system becomes instable. And that will be the sufficient condition for the instability; you do not require any more condition to check the instability. If one of the eigenvalues will be having a real part above 0 greater than positive, then will be having an instable solution.

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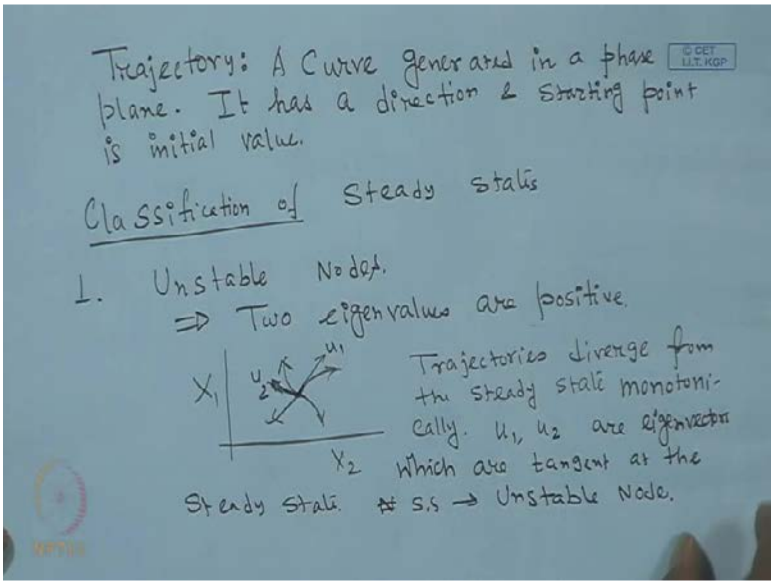

Next, we will look into some of the definitions, first one is called a trajectory; trajectory is a curve generated in a, curve generated in a phase plane that is called a trajectory. It has a direction starting with the initial value, it has a direction and the starting point is the initial value. Now, next we classify the various steady; so, classification of steady states these are quite important and you come across of several terms later on, that is the unstable saddle, unstable node, focus, stable focus, unstable focus, so on so forth.

So, let us classify the steady states, the first classification is the unstable nodes. If two Eigenvalues are positive unstable nodes occurs that when two Eigenvalues are positive. And the phase plane plot looks something like this, so you will be having an initial condition here. Then, so, any deviation in about the initial condition, it will diverge from this steady state and this node is called an unstable nodes and this will be the direction of the Eigenvectors, the tangential directions presented in the node at the Eigenvectors.

So, therefore trajectories diverge from the steady state monotonically, so that is the feature of unstable node. So, u 1, u 2 are the Eigenvectors; so, these are the direction of the Eigenvectors; u 1, u 2 are Eigenvectors which are tangent at the steady state, such kind of node or steady state is called unstable node. So, because of the presence of unstable node, any steady state around this point will diverge from this steady state. So these are called unstable nodes.

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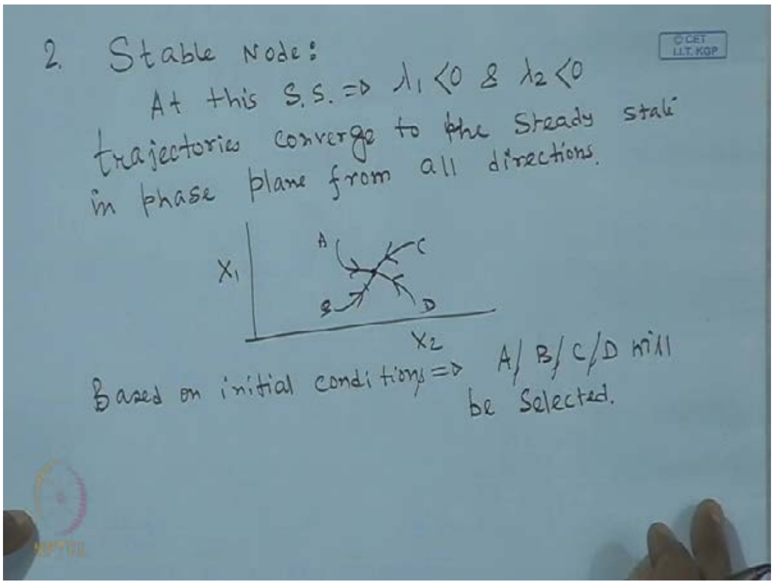

Then we talk about a stable node that is the second type of steady. State stable node is this at this steady state, both Eigenvalues are negative; so, lambda 1 is negative and as well as lambda 2 is negative; so, that means, the trajectories converge to the steady state in phase plane from all direction, then, that particular node is called stable node. And if you look into the phase plane plot, so it will be x 1 versus x 2 and if this is the steady state any steady state, around this point will converge to this, but which steady state… Now, suppose A, B, C, D, now which trajectory it will follow, suppose you have a steady state here and we have a point around the steady state, from this point now it will be following this.

Now, based on the initial condition it will decide which steady state which path it will take up. So, based on initial condition, based on the initial conditions the path A, B, C or D will be selected, so that is called a stable node; that means, in case of stable node, we have the Eigenvalues less than 0; that means, both of the Eigenvalues are negative and one can have a very stable system in around that point, so any deviation about the steady state we will lead to the particular steady state, so then it is called a stable node.

In case of a system, where one of the Eigenvalues is positive, then you will be having the any deviation from the steady state will lead to divergence from that particular solution. If all steady states, if all Eigenvalues are positive, then that will be an unstable steady state, so it will be an unstable node. So, any definition from any direction of the steady state, it will diverge from the steady state. In the next class, I will stop here at this class, in the next class, will look into some more definitions of the steady state and we will complete the classification of the steady state, then we go to the appropriate examples and further develop the theory and finally so will take up some of the examples of chemical engineering system.

Thank you very much.