

**Mathematical modelling and Simulation of Chemical Engineering Process**  
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**Lecture 19**  
**Stability of dynamical systems**

Hello everyone, Stability of a Dynamic Process is very important in Chemical Engineering Systems, you might have encountered stability issues for control of steady state reactor, it could be control of a runaway or autocatalytic reaction or it could be any control systems where there is a possibility of multiple steady states and you need to determine that your system, will be stable or unstable at a particular steady state. So, this analysis of stability is very crucial and this is often helpful from operational perspective as well as design of effective control systems.

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The banner features a blue and black geometric design at the top. On the left is the NPTEL logo, a stylized flower-like shape with yellow and red petals. On the right is the IIT Kharagpur logo, a circular emblem with a tree and the motto 'योगः कर्मसु कौशलम्'. Below the logos, a blue banner contains the text 'NPTEL ONLINE CERTIFICATION COURSES'. The main text of the banner reads: 'Mathematical modelling and simulation of chemical engineering process', 'Dr Sourav Mondal', 'Chemical Engineering, IIT KHARAGPUR', and 'Lecture 19 : Stability of dynamical systems'.

## CONCEPTS COVERED

- ❖ Application of stability in ChE problems
- ❖ Stability criterion in lumped systems



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Now, in this lecture today, we are going to talk about stability of, and we are going to analyze in fact the stability criteria of chemical engineering process and try to frame the generic stability criteria which is applicable for lumped systems and possibly in the next class we will talk about further deep into the bifurcation analysis and about stability in distributed parameter system. But in this lecture, we are going to focus on the criteria for the stability and how it is actually evolved.

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Non-isothermal CSTR, 1st order reversible reaction

$$\text{(terms)} \frac{dc}{d\tau} = -c + Da(1-c)e^T$$

$$\text{(terms)} \frac{dT}{d\tau} = -(1+\beta) + BDa(1-c)e^T$$

$$\text{At. ss.} \quad \frac{dc}{d\tau} = 0 \equiv \boxed{-c + Da(1-c)e^T = 0}$$

$$\frac{dT}{d\tau} = 0 \equiv \boxed{-(1+\beta) + BDa(1-c)e^T = 0}$$

Eliminate T



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But first we are going to start with a small example of where the stability is critical in chemical engineering systems. So, let us say you have a Non-isothermal CSTR with first order reversible reaction. So, you can look into any Chemical Engineering Reaction Engineering book. And let us say well I am writing the solute balance and temperature balance in sort of a dimensionless form, where I think all of you realize that this Damkohler number is a mixing parameter in the CSTR and so, the top is the solute balance and next I am writing the temperature balance from the enthalpy balance of the process.

So, this Beta and this B all are certain constants of the process you can think of them to be some sort of either a summation or a compounded reaction constants or the volume space time and all those things of course, on all both of these equations on the left hand side there are few terms which I am just in, I have not written down just for the sake of simplicity in analysis.

Now, these two equations on t is the Tau, whatever you have written is the non dimensional time, that is Non-dimensionalized are scaled with respect to a time scale of the problem. Now, at steady state both of these dC, dTau would be equal to 0 which implies that minus C plus D a this is equal to 0, as well as this enthalpy equation is also 0, which implies you have minus 1 plus Beta.

So, these two are the equations which is obtained at the steady configuration. Now, please have a critical look into this two equations, these two equations are of course composed of the process variables that is a T and coil temperature and the concentration. So, let us say if I wanted to eliminate, let us say I wanted to eliminate just a small substitution eliminate T from the above two equations.

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$f(c) \equiv Da = \frac{c}{1-c} \exp\left(-\frac{BC}{1+\beta}\right)$

$f(c) = \frac{c}{1-c} \exp\left(-\frac{BC}{1+\beta}\right)$

$f'(c) = 0$  condition for max. & min.

$\beta c^2 - BC + (1+\beta) = 0$

$c_{1,2} = \frac{B \pm \sqrt{B^2 - 4B(1+\beta)}}{2B}$

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To have real roots,

$$B^2 - 4B(1+\beta) > 0$$

$$\Rightarrow B > 4(1+\beta)$$

$$B > 1+\beta$$

$$B < 1+\beta$$

The graph plots concentration  $C$  on the vertical axis against the Damkohler number  $Da$  on the horizontal axis. Two curves are shown. The upper curve, labeled  $B > 1+\beta$ , starts at the origin and increases monotonically. The lower curve, labeled  $B < 1+\beta$ , starts at the origin, increases to a peak, then decreases to a minimum, and finally increases again, forming a hysteresis loop. A vertical dashed line intersects the lower curve at two points, indicating multiple possible concentration values for a single Damkohler number.

Then the equation that we are going to get will look something like this, with only the variation in the  $C$ . So, let us call so, this concentration is related to the Beta  $B$  and the Damkohler numbers let us call this as a function of  $C$ , let us call the right hand side, this right hand side of this equation as a function of  $C$ . So, if I am going to plot this  $C$  versus Damkohler number I am going to get something like this.

So, for every value of Damkohler number, there is a possibility of a unique value of the  $C$ . Now, there is also a possibility that it may not be true always, it may not be true always that the curve of  $Da$ , versus  $C$ , looks like a monotonically increasing or like a unique value 1 to 1 mapping, it could be possible that this curve looks something like this, where for a particular value of a Damkohler number there is a possibility of existence of multiple  $C$ .

So, under what circumstances this is possible, let us investigate this further, let us say, I write this  $f(C)$  once again, I take the derivative of this and if I set the derivative to be 0, this is the condition for maxima and minima.

So, if we find that there is a possibility of a maxima and minima, then it is most likely that the curve is not a monotonic function there is a presence of multiple values of  $C$  for a particular value of the Damkohler number. So, if you do the this derivative you get, I mean the first derivative something like this and this you can set the values of, I mean this is a parabola sorry, this is a quadratic equation so, you can get two values of your concentration that is plus

minus something like  $B^2 - 4B + \beta$  and you can clearly see that to have real roots from this equation to have real roots you will need to satisfy these criteria.

So, which means  $B$  has to be greater than  $4 + \beta$  for this condition to be feasible or to have real roots. So, typically if I tried to draw the two curves, let us say  $C$  versus  $D$ . So, this would be the case when  $B$  is less than  $1 + \beta$  and this would be the case when  $B$  is greater than  $1 + \beta$  or there is an existence of two possible values of your  $C$  and of course, one could be maximum, one could be minimum. So, these and all of these values please remember this  $C$  is nothing but the steady state  $C$ .

So, there is a possibility of having two steady state in the problem and possibly one of them is stable and one of them could be unstable who knows. So, there lies the need for the inspection of the stability of dynamical systems.

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System of ODEs,

$$\frac{dx_1}{dt} = \dot{x}_1 = f_1(x_1, x_2)$$

$$\frac{dx_2}{dt} = \dot{x}_2 = f_2(x_1, x_2)$$

Step I: Identify the SS

$$\dot{x}_1 = \dot{x}_2 = 0 \Rightarrow \left. \begin{array}{l} f_1(x_1^*, x_2^*) = 0 \\ f_2(x_1^*, x_2^*) = 0 \end{array} \right\} \begin{array}{l} F(x^*) = 0 \text{ where} \\ x^* = [x_1^* \ x_2^*]^T \end{array}$$

$\dot{X} = F(X)$  where  $X = [x_1 \ x_2]^T$   
 $F = [f_1 \ f_2]^T$

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So, let us consider as we say that in this class we are focusing mostly on the case of lumped system. So, we will be dealing with system of ODEs. Let us say we have two ODEs governing of the system and the state variable let us define that as  $x_1$  and  $x_2$  in this way.

So, I define two equations for each case, for each of the state variables. So, I can also write this in the, in a sort of a matrix form like  $\dot{X}$  is equal to some like function of  $X$  where  $\dot{X}$

and at the top of it represents its, the temporal derivative. So, I can consider this is like a state space vector.

Similarly F is f1, f2. So, what is the first step in the analysis of this stability or to work on the analyzing them and to derive the condition for the stability, first is to identify the steady state. So, what is this case here that both x1 dot, x2 dot both will be set to 0 and under these conditions we will be getting let us say I represent the x1 variable is steady state as x1 star. So, both of these variables at the steady state level is represented by x1 star, x2 star. So, similarly I can write the vector form like this. So, once you do this step the next step is the linearization part.

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II Linearization:

$x_1 = x_1^* + \varepsilon \tilde{x}_1(t)$

$x_2 = x_2^* + \varepsilon \tilde{x}_2(t)$

So,  $x = x^* + \varepsilon \tilde{X}(t)$  where  $\tilde{X} = [\tilde{x}_1 \ \tilde{x}_2]^T$

Perturbation of small  $\varepsilon$  around the ss

$\frac{dx_1}{dt} = f_1(x_1, x_2) \rightarrow \frac{dx_1}{dt} = \frac{dx_1^*}{dt} + \varepsilon \frac{d\tilde{x}_1}{dt}$

$\Rightarrow \varepsilon \frac{d\tilde{x}_1}{dt} = f_1(x_1^* + \varepsilon \tilde{x}_1, x_2^* + \varepsilon \tilde{x}_2)$

$= f_1(x_1^*, x_2^*) + \varepsilon \tilde{x}_1 \left. \frac{\partial f_1}{\partial x_1} \right|_{x_1^*, x_2^*} + \varepsilon \tilde{x}_2 \left. \frac{\partial f_1}{\partial x_2} \right|_{x_1^*, x_2^*}$

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$$\begin{aligned} \varepsilon \frac{d\tilde{x}_2}{dt} &= f_2(x_1^* + \varepsilon\tilde{x}_1, x_2^* + \varepsilon\tilde{x}_2) \\ &= \underbrace{f_2(x_1^*, x_2^*)}_{=0} + \varepsilon\tilde{x}_1 \left. \frac{\partial f_2}{\partial x_1} \right|_* + \varepsilon\tilde{x}_2 \left. \frac{\partial f_2}{\partial x_2} \right|_* \end{aligned}$$

$$\text{So, } \begin{aligned} \dot{\tilde{x}}_1 &= \left. \frac{\partial f_1}{\partial x_1} \right|_* \tilde{x}_1 + \left. \frac{\partial f_1}{\partial x_2} \right|_* \tilde{x}_2 \\ \dot{\tilde{x}}_2 &= \left. \frac{\partial f_2}{\partial x_1} \right|_* \tilde{x}_1 + \left. \frac{\partial f_2}{\partial x_2} \right|_* \tilde{x}_2 \end{aligned} \Rightarrow \dot{\tilde{X}} = \underline{\underline{J}} \tilde{X}$$

$$\underline{\underline{J}} = \begin{bmatrix} \left. \frac{\partial f_1}{\partial x_1} \right|_* & \left. \frac{\partial f_1}{\partial x_2} \right|_* \\ \left. \frac{\partial f_2}{\partial x_1} \right|_* & \left. \frac{\partial f_2}{\partial x_2} \right|_* \end{bmatrix}_{x_1^*, x_2^*}$$



So, what is linearization? So, this is step 2, so in linearization we choose a small perturbation of the state variable  $x_1$  around its steady state. So, this is a small perturbation in the order of epsilon scale, we add to the variable I mean to the, to the variable at the steady state to define my state variable  $x_1$  and similarly,  $x_2$  can also be defined in the same way.

So, this is a small perturbation which is added to the state variable and then we are going to work out in terms of the the first order Taylor expansion of this epsilon we are going to do a balance of the perturbation technique, which is something which you have already studied in the previous lectures. So, so, this is this epsilon is perturbation of small epsilon around the steady state.

So, similarly, I can write in terms of the vector or the matrix formulation capital  $X$  like this where, now, let us substitute these equations into the main governing equations. So, if I take the derivatives on both sides, what is going to appear here and we are going to use them back to our original equation and a steady state.

So, if I try to do this that is  $dx_1/dt$  something like this we are going to try to work out which is equal to let us say  $f_1, x_1$  comma  $x_2$  the same thing if we are going to do what we will be getting here is something like this, because please note that  $x_1$  star is the steady state value. So, if I take the derivative of  $x_1$  star with respect to time that is going to be 0.



Similarly, if I do the derivative of  $\frac{dx_1}{dt}$  at steady state that is also going to be 0, that is what we started off initially. So, from both the sides I am going to get sorry, this  $\frac{dx_1}{dt}$  will be equal to  $f_1$ ,  $f_1$  of  $x_1$ ,  $x_2$  and that is what I am writing, trying to write here. So, what we did is that, we did the simply differentiation from this equation. We actually tried to do a differentiation here on both sides. So, what we did is  $\frac{dx_1}{dt}$  derivatives on both sides, so, this is equal to 0 because this is a steady state and this is equal to  $f_1$  and this is what we got this equation from.

So, if I try to expand this, so, these right-hand side can be expanded as a Taylor series function. So, what is the Taylor series function,  $f_1(x_1^*, x_2^*) + \epsilon x_1 \frac{df_1}{dx_1}$  at  $x_1^*$   $x_2^*$  plus  $\epsilon \frac{df_1}{dx_2}$  at the star conditions and please note that this term is equal to 0, is not it?

So, we have only this term and another term is this, same thing we can do it for the  $\frac{dx_2}{dt}$ , let us do it out. So,  $\epsilon \frac{dx_2}{dt}$  will be  $f_2$  sorry this is  $x_1$ . So, we do the same Taylor series expansion here  $x$  plus  $h$ , sorry here should be one epsilon, and both of them are evaluated steady state conditions and this one is equal to 0.

So, what I can, what I see here is this if I ignore the epsilons I mean on both sides what I get here, this is equal to  $\frac{df_1}{dx_1}$  and which is multiplied to  $x_1$  plus  $\frac{df_1}{dx_2}$  multiplied with the part of the variable. Similarly, this equation can also be written down as, so, here once again I can get the vector form.

So, and where is this what is this  $J$ ? So,  $J$  is nothing but the Jacobian, is not it, of the two functions with respect to each of the state space vectors. Which is of course evaluated at  $x_1^*$  and  $x_2^*$ , that is at the steady state. I hope this is clear to everyone till this part. Now the next step is to work out by adding a small growth rate parameter.

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Step III  $\dot{\tilde{x}} = \underline{J} \tilde{x}$  if  $\frac{dy}{dt} = \sigma y$   
 $y = y(0) e^{\sigma t}$

disturbance  $\tilde{x}_1(t) = u_1 e^{\sigma t}$  growth rate  
 $\tilde{x}_2(t) = u_2 e^{\sigma t}$

$\sigma > 0$  perturbations will grow with  $t$   
 $\sigma < 0$  perturbations will be suppressed

$\sigma u_1 e^{\sigma t} = \frac{\partial f_1}{\partial x_1} \Big|_* u_1 e^{\sigma t} + \frac{\partial f_1}{\partial x_2} \Big|_* u_2 e^{\sigma t}$   
 $\tilde{x}_1 = \frac{\partial f_1 / \partial x_1}{\sigma} \tilde{x}_1 + \frac{\partial f_1 / \partial x_2}{\sigma} \tilde{x}_2$

So, this is step 3. So, here so, we already have this equation. So,  $\tilde{x}$  or  $\bar{x}$  is the perturbation vector and we got this equation,  $J$  is the Jacobian here now, let us see that this how this small perturbation  $x_1(t)$  is going to vary. So, this is something like going to vary in this form.

So, this  $\sigma$  is the growth rate of the disturbance. So, this  $x_1$  is nothing but a sort of disturbance in the manipulated variable to the process variable and let us say that process variable disturbance varies exponentially with time with a growth rate. Now, how generally how this thing actually came to the existence that if this let us say we call this that if this perturbation or this disturbance follows a first order state system then essentially you are going to get something like this.

So, considering let us say the  $y$  is a disturbance and generally the disturbance can be assumed in the first case to be following a first order nature then the growth rate of a disturbance is exponential in nature. Now, the condition is that if the growth rate  $\sigma$  is negative then this disturbance will actually reduce in time and after finite time it will be very small the disturbance will actually be suppressed, but if this  $\sigma$  is positive then the disturbance will grow and ultimately make the system stable, unstable.

So, similarly, we can write this for  $x_2$ . So, in both the cases we choose the same growth rate, this is sort of an assumption and this generally holds true for most cases if there is a disturbance or a fluctuation in one of the process variable at a certain growth rate the disturbance is changing then it will also affect the other process variable at the same rate, but this is to some extent an assumption. So, if  $\sigma$  is greater than 0 then the perturbations will grow with time and if it is less, then the perturbations will be suppressed.

So, now, with these two descriptions of the, sorry with two descriptions of the disturbance we are going to feed them into the main equation. So, these two equations whatever we have here, we will try to feed them into the main equation and try to get an estimate on this  $\sigma$ . So, that is step 3 essentially we are just extending this here.

So, let us write it down so, we have  $\sigma u_1 e^{\sigma t}$  to the power  $\sigma t$ ,  $df_1/dx_1$ ,  $u_1 e^{\sigma t}$  to the power  $\sigma t$ , plus  $df_1/dx_2$   $u_2 e^{\sigma t}$  to the power  $\sigma t$ . Is it not, it so, what is what I have written now? So, this is  $x_1$  sorry this dot then  $df_1/dx_1$  this is  $x_1$  plus  $df_1/dx_2$  this is  $x_2$  this is the equation which I have just substituted the values of  $x_1$  in the form of  $u_1 e^{\sigma t}$  to the power  $\sigma t$ . So, this is what the derivatives looks like. So, this term is represented here and this term is represented here.

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$$\sigma u_1 e^{\sigma t} = \left. \frac{\partial f_1}{\partial x_1} \right|_{x^*} u_1 e^{\sigma t} + \left. \frac{\partial f_1}{\partial x_2} \right|_{x^*} u_2 e^{\sigma t}$$

$$\sigma u_2 e^{\sigma t} = \left. \frac{\partial f_2}{\partial x_1} \right|_{x^*} u_1 e^{\sigma t} + \left. \frac{\partial f_2}{\partial x_2} \right|_{x^*} u_2 e^{\sigma t}$$

$$\therefore \sigma U = J U \quad \text{where } U = [u_1 \ u_2]^T$$

Eigen value problem.

Step IV: Solve the EVP

$$\sigma U = J U \Rightarrow [J - \sigma I] U = 0$$

$$\det [J - \sigma I] = 0 \quad \text{characteristic equation.}$$

Calculate  $\sigma$  from  $\det [\underline{I} - \sigma \underline{I}] = 0$   
 $\sigma \rightarrow$  eigen values.  
 $\text{Re}(\sigma) > 0$  system is unstable.  
 $\text{Re}(\sigma) < 0$  stable.

So, similarly, I can also write the second case also, sorry, I will rewrite it once again here, this is for the case of  $x_1$  and here we are getting for the case of  $x_2$ . Sorry this is  $u_1 e$  to the power  $t$ . So, on both sides we can cancel  $e$  to the power  $\sigma t$ . And then what you get  $\sigma u_1$ . So, I can directly write I think all of you are quite mature enough at this stage that I can directly write this one in the vector form, is it not? and yes, so, this is the eigenvalue problem of the disturbance.

Now, we try to solve the eigenvalue problem that is step number 4 and the final step solve the eigenvalue problem and find out it find out its Eigen values. So, this is the Eigen value problem. So, to solve the eigenvalue problem, you know that what we need to do is that we need to bring both of these things in one side so, I get something like this.

So, clearly  $U$  is not equal to 0. So, we set determinant of this to be equal to 0. So, this is the characteristic equation and the characteristic equation of this determinant will give me the Eigen values and Eigen values are nothing but my  $\Sigma$ , is it not? So, the criteria say that you obtain or calculate  $\sigma$  from this, the characteristic equation.  $J$  is a matrix and  $I$  is the identity matrix from here, you calculate this  $\sigma$ .

So, if this  $\sigma$  and  $\sigma$  are the Eigen values essentially. So, if the real part of the Eigen value if it is positive then system is unstable. No more conditions are required, system is

simply unstable and if real part of the sigma is less than 0 system is stable but there are further analysis is needed that what happens to the imaginary conditions.

So, the important part is that if the sigma or this disturbance is less than 0 essentially the real part of the sigma from this characteristic equation is less than 0, it may have n number of Eigen values. So, in this case it will have two Eigen values because we are dealing with two state variables, but for more number of state variables it can have n number of solutions. So, even if one of the solutions of the, if one of the Eigen value is positive or the real part is positive essentially it will lead to instability of the system.

So, for stability it is very essential that the real component of the eigenvalues which is essentially the growth rate in this case is less than 0. So, I hope all of you have got the idea of the condition for which stability is determined. Eigen values play a very critical role here for the eigenvalue problem. And in the next class we are going to talk about the further analysis into this stability and then we look into the stability for distributed parameter system. I hope all of you have liked this lecture and you found it useful. Thank you.