Advanced Process Dynamics

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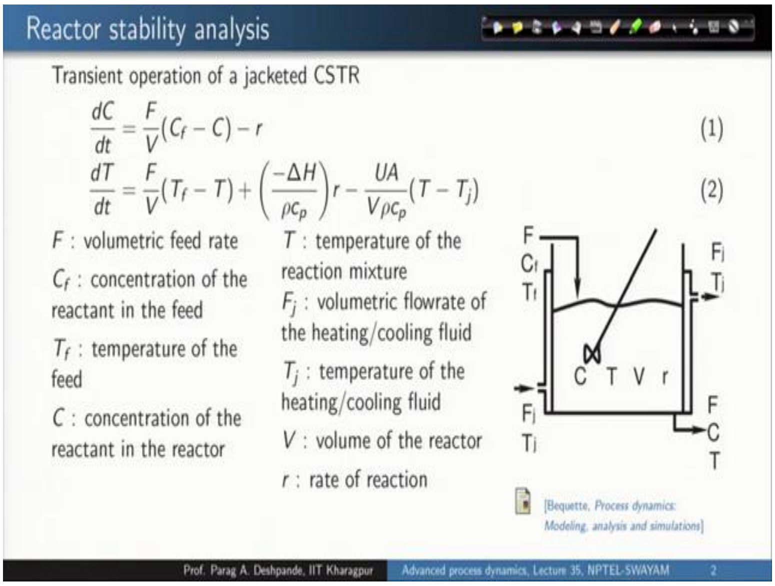
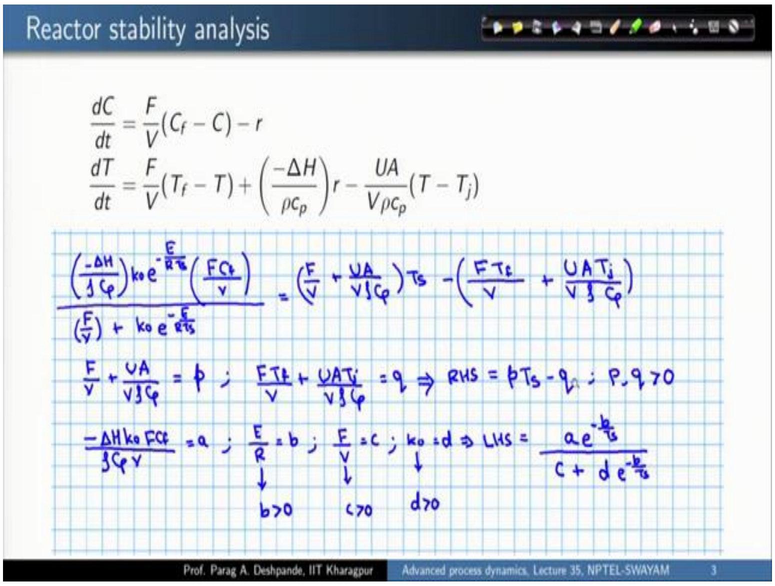
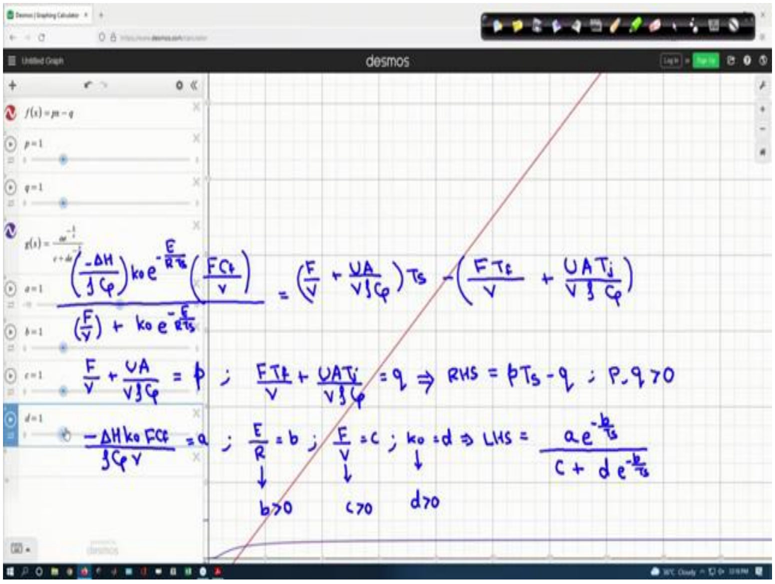
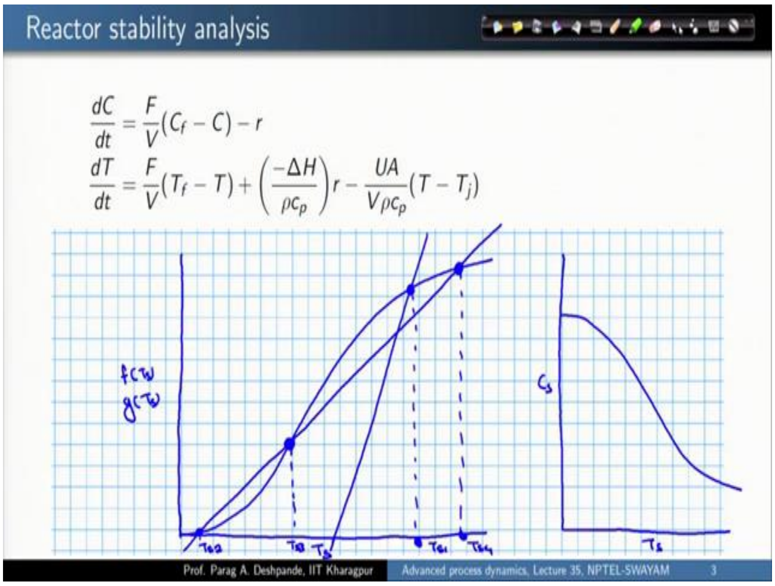
Lecture 35

Reactor Stability Analysis (Continued)






desmos
Untitled Graph
$f(x) = px - q$
$p = 1$
$q = 1$
$g(x) = \frac{ae^{-\frac{b}{x}}}{c + de^{-\frac{b}{x}}}$
$a = 1$
$b = 1$
$c = 1$
$d = 1$
$\frac{\left(\frac{-\Delta H}{\rho C_p}\right) k_0 e^{-\frac{E}{RT_s}} \left(\frac{F C_f}{V}\right)}{\left(\frac{F}{V}\right) + k_0 e^{-\frac{E}{RT_s}}} = \left(\frac{F}{V} + \frac{UA}{V\rho C_p}\right) T_s - \left(\frac{F T_f}{V} + \frac{UA T_j}{V \rho C_p}\right)$
$\frac{F}{V} + \frac{UA}{V\rho C_p} = p \; ; \; \frac{F T_f}{V} + \frac{UA T_j}{V\rho C_p} = q \Rightarrow RHS = pT_s - q \; ; \; p, q > 0$
$\frac{-\Delta H k_0 F C_f}{\rho C_p V} = a \; ; \; \frac{E}{R} = b \; ; \; \frac{F}{V} = c \; ; \; k_0 = d \Rightarrow LHS = \frac{a e^{-\frac{b}{T_s}}}{c + d e^{-\frac{b}{T_s}}}$
$b > 0$
$c > 0$
$d > 0$


Reactor stability analysis
$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r$
$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right) r - \frac{UA}{V\rho c_p}(T - T_j)$
f(T)
g(T)
T_{s2}
T_{s3}
T_s
T_{s1}
T_{s4}
C_s
T_s
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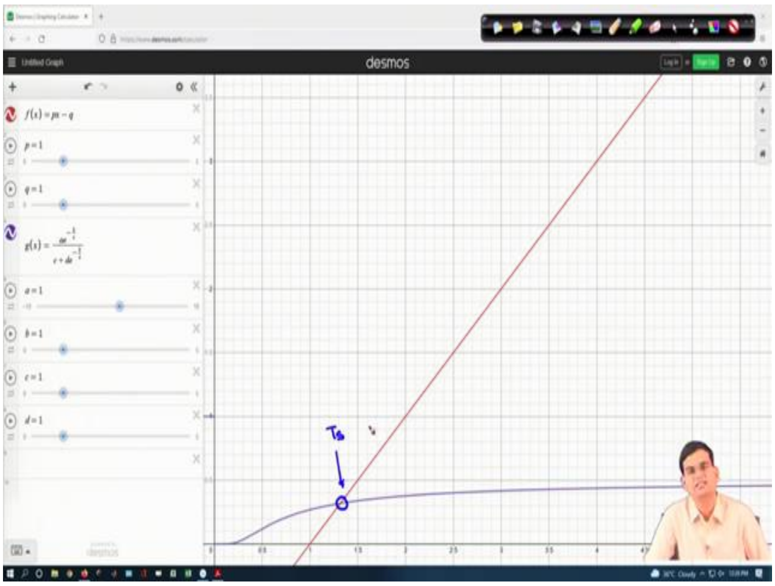
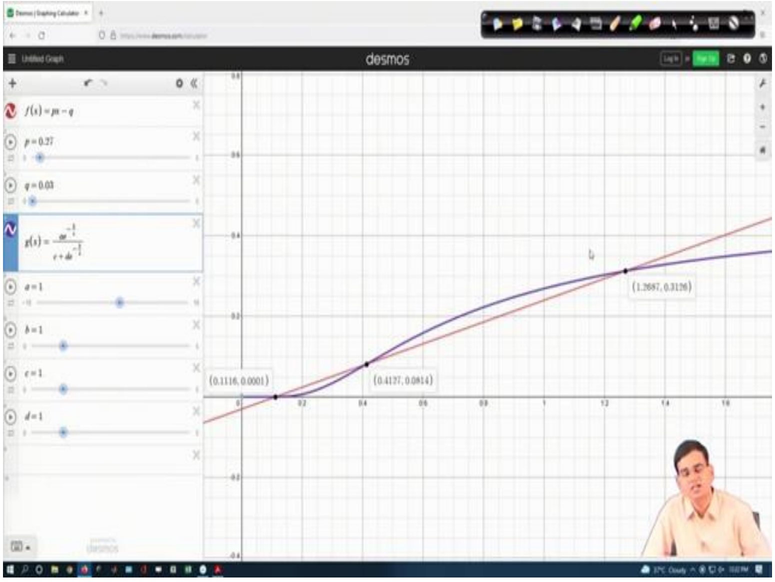
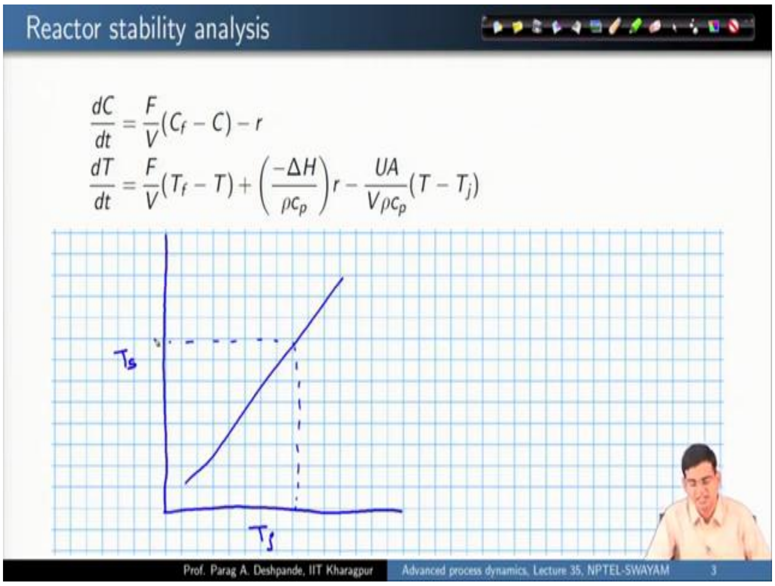

desmos
Untitled Graph
$f(x) = px - q$
$p = 1$
$q = 1$
$g(x) = \frac{ae^{-\frac{b}{x}}}{c + de^{-\frac{b}{x}}}$
$a = 1$
$b = 1$
$c = 1$
$d = 1$
T_s


desmos
f(x) = px − q
p = 0.27
q = 0.03
a = 1
b = 1
c = 1
d = 1
(0.1116, 0.0001)
(0.4127, 0.0814)
(1.2687, 0.3126)


Reactor stability analysis
$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r$
$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right) r - \frac{UA}{V \rho c_p}(T - T_j)$
T_s
T_j
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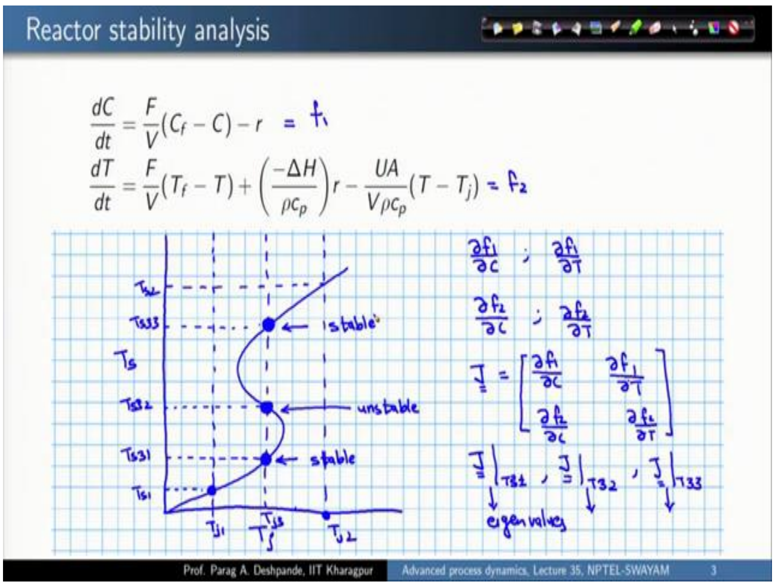
Reactor stability analysis
$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r = f_1$
$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right) r - \frac{UA}{V \rho c_p}(T - T_j) = f_2$
T_{s2}
T_{s33}
T_s
T_{s32}
T_{s31}
T_{s1}
stable
unstable
stable
T_{j1}
T_{j3}
T_j
T_{j2}
$\frac{\partial f_1}{\partial C}$; $\frac{\partial f_1}{\partial T}$
$\frac{\partial f_2}{\partial C}$; $\frac{\partial f_2}{\partial T}$
$\underline{\underline{J}} = \begin{bmatrix} \frac{\partial f_1}{\partial C} & \frac{\partial f_1}{\partial T} \\ \frac{\partial f_2}{\partial C} & \frac{\partial f_2}{\partial T} \end{bmatrix}$
$\underline{\underline{J}}\big|_{T_{S1}}, \underline{\underline{J}}\big|_{T_{32}}, \underline{\underline{J}}\big|_{T_{33}}$
eigenvalues
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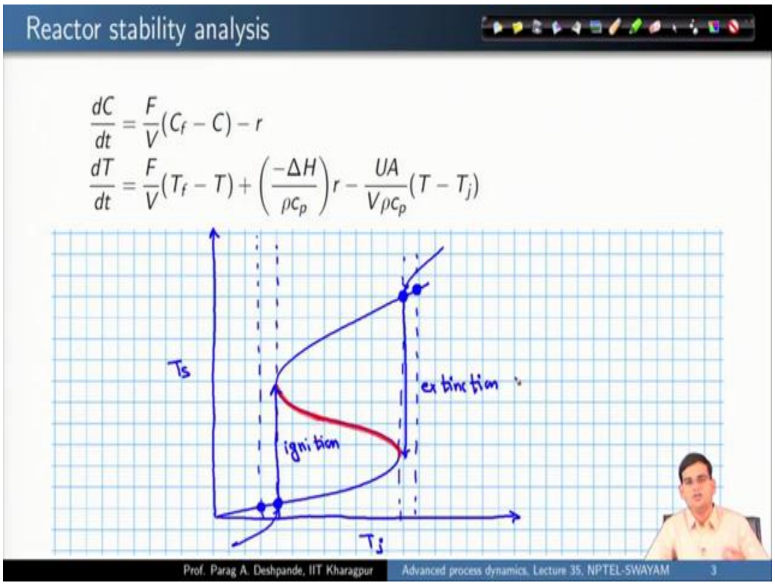

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Let us continue our discussion on reactor stability analysis, we discussed the steady state solution for concentration profile and then we got a complex expression for steady state profile for temperature. So, the equations were like this and when we solve for steady state temperature what we got was an expression of this form

$$\frac{\left(\frac{-\Delta H}{\rho c_p}\right) k_0 e^{-\frac{E}{RT_s}} \left(\frac{FC_{fs}}{V}\right)}{\frac{F}{V} + k_0 e^{-\frac{E}{RT_s}}} = \left(\frac{F}{V} + \frac{UA}{V\rho c_p}\right) - \left(\frac{FT_f}{V} + \frac{UAT_j}{V\rho c_p}\right)$$

So, this was the expression that we had in front of us. Then we said that in order to determine the steady state temperature we need to individually draw say the graphs of the left-hand side and the right-hand side and the point of intersection would be the steady state temperature.

Let us see what kind of functions are these, let us first look at the the right-hand side. Now, $\frac{F}{V}$ is a constant, F is a constant, V is a constant. U, A, ρ, Cp...... all of these are constants. So, let me say that

$$\frac{F}{V} + \frac{UA}{V\rho c_p} = p$$

Further everything is the system is assumed to be at steady state so feed rate would be constant, temperature of the feed would be constant, the material properties have been assumed to be constant, so U, A, V, ρ, Cp....... everything would be a constant.

So therefore, I can write

$$\frac{FT_f}{V} + \frac{UAT_j}{V\rho c_p} = q$$

So therefore, in light of this the right-hand side would be

$$RHS = pT_s - q$$

and what kind of function is this, this is simply a linear function with p and q as constants. So not very difficult to see that you would have simply, and what kind of quantities would p and q be, F, V, U, A, ρ, Cp........ are all positive. So, p would be positive, similarly F, T_f, V, U, A, T_j, ρ, V, Cp....... are all positive. So, therefore p as well as q would be positive.

So,

$$p, q > 0$$

Let me plot this and see the nature so,

$$f(x) = px - q$$

Not very difficult to see how this plot would look like and we would also set p and q between 0 and 5 to confirm that they are positive 0 and 5. Now what about the other quantity? So, the left-hand side now

$$\frac{-\Delta H k_0 F C_f}{\rho c_p V} = a$$

Let me call

$$\frac{E}{R} = b; \ \ \frac{F}{V} = c; \ \ k_0 = d$$

So, this will make the left-hand side what?

$$LHS = \frac{ae^{-\frac{b}{T_s}}}{c + de^{-\frac{b}{T_s}}}$$

So let me try to plot this function now,

$$g(x) = \frac{ae^{-\frac{b}{x}}}{c + de^{-\frac{b}{x}}}$$

Now let us also analyze what kind of quantities these are. So,

$$\frac{E}{R} = b > 0; \quad \frac{F}{V} = c > 0; \quad k_0 = d > 0$$

Now, rest all the quantities in a, so k_0, FC_f, ρ, Cp, V...... are positives but ΔH depending upon exothermic or endothermic may be positive or negative. So, let us for sure set b as positive, c as positive and d as positive. Now I see that the intersection of the two curves so the intersection of $LHS = \frac{ae^{-\frac{b}{T_s}}}{c+de^{-\frac{b}{T_s}}}$ and a straight line given as $RHS = pT_s - q$ should give me the steady state, let us see if this is correct.

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So, let me do one thing this is f and this is T_s......f or g in fact, so let me look into this let me zoom in. I will be interested only in the first quadrant but let me zoom in; so that I will be able to have a look into this better. So now what I see is that I have the left-hand side involving exponential so you have this non-linear curve I have the right-hand side which is a straight line you get this and then you get one point of intersection and therefore this is your T_s. So, you fix the flow rate, you fix the feed concentration, you fix the jacket flow rate, you fix the jacket temperature you get one steady state looks very simple....... very trivial in fact. Let me now do a small arrangement with the parameters of the system, and let me then see if I see something very different and in fact something very interesting so let me try to change the parameters and what I will do is I will change the value of p and q.

Let us see what I have done. So, I will zoom in further and what I see is that instead of one intersection which you would expect to be a unique solution for your system as the steady state temperature, now you have three points of intersection so what are the three points of intersection; point 1, point 2, point 3, the absolute values do not have any significance here because you will punch in various values of heat transfer coefficient, flow rates etc. What I want to show you here is that you in fact have three steady state temperatures. Now the question is how you can have three steady state temperatures for the same state of your system, same flow rate, same temperature, feed temperature, same jacket temperature and so on; well because the system is non-linear.

So, since the system is non-linear now you have the intersection of your heat generation curve which is a non-linear curve with your heat removal curve which is a straight line. So, we would be interested in knowing the natures of these solutions, so let us clearly point out that you have 1, 2 and 3; in fact, there can be three intersection points corresponding to three solutions, they can be two, they can be one.

So now if I draw the general trend of this equation here what I see is this, so this is steady state temperature this is function $f(T_s)$, $g(T_s)$, one of them is a straight line. I know but the other one look like this. In one case you had one intersection point which is like this and therefore you have a unique steady state and what is the importance of this unique steady state, T_{s1}?

The importance of this unique steady state is that well it makes your life easy because you know that I have set my feed temperature, I have set my feed concentration, I have set my temperature of the jacket, so I will calculate and I can know what would be my steady state reaction which temperature very simple. Now I have a case where you have three intersection points 1, 2, and 3, so T_{s2}, T_{s3} and T_{s4}. So, for the same input flow rate, for the same flow rate of jacket fluid, or the same temperature of jacket fluid, for the same feed concentration, for the same feed temperature and all the material properties, now you have three steady state solutions and therefore it becomes imperative to know that if I am going to give the same values of the parameter where am I going to land up?

Because previously we saw that the variation of the concentration with steady state temperature, so this is this steady state temperature, this is the steady state concentration look like this. So therefore, when you want to know the steady state concentration you would like to know the steady state temperature, but now instead of one temperature I have three temperatures and therefore I must know how much is the output which I am going to get from my system. Now there is an ambiguity, so what we will need to do is we will need to analyze the stability of these points? Before we do that what we also need to do is this that if you have well you got this curve by an intersection of the f function which was nothing but the heat removal, your g function which was nothing but heat generation and you try to determine the intersection. If you rearrange these equations, you can as well draw several other graphs.

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One of the graphs for example would be this T_j versus T_s here; in general, what would you expect? Well, if I set some flow rate of the fluid in the jacket and that jacket fluid has some temperature then because of the heat exchange at steady state I must get one unique value of the steady state temperature inside the reactor. So, what you should expect is that as my jacket temperature goes on increasing, my steady state temperature should go on increasing, some kind of a pattern like this.

So for a jacket temperature you get a unique steady state temperature, but that does not happen in fact the way we plotted the previous plot if you rearrange everything as a function of steady state temperature on one side and jacket it on the other side what you will get is what you will observe is that you in fact get a curve which looks like this, so let me draw the curve which you will get from a similar analysis I am leaving the analysis for you I am leaving the rearrangements for you to do the nature of the curve and if you put that in decimals you will get this kind of a curve the curve looks like this its an S shaped curve.

So now what is the problem with this curve you would be operating your system at certain jacket temperature, so let me draw three vertical lines so these are the operational lines, so if I drop the first vertical line here, I get this intersection which means that for this jacket temperature T_{j1}, I will get this steady state temperature T_{s1}.

Similarly, I drop this another operational vertical line for T_{j2}, I get this steady state temperature again not a problem T_{s2}, one jacket temperature one steady state temperature that is fine. Now let us have a look into this T_{j3}, for T_{j3} you have T_{s3}.

You have three steady state temperatures, but we have previously seen that it is possible that you get multiple solutions but all of them may not be stable, so if you have one particular solution which is unstable then you would not physically observe that solution and therefore it is okay, you need to worry about only the stable solutions, how would you get an idea whether a solution is stable or unstable in all of these cases?

Well, what you will do is you will linearize your system, so how would you linearize your system I will assign this as function f or f_1 rather;

$$\frac{dC}{dt} = \frac{F}{V}\left(C_f - C\right) - r = f_1$$

I will assign this as function f_2.

$$\frac{dT}{dt} = \frac{F}{V}\left(T_f - T\right) + \left(\frac{-\Delta H}{\rho c_p}\right) r - \frac{UA}{V\rho c_p}\left(T - T_j\right) = f_2$$

So, this is an exercise which I am leaving you to do; what you will do is you will do

$$\frac{\partial f_1}{\partial C};\ \frac{\partial f_1}{\partial T}$$

Similarly, you will determine

$$\frac{\partial f_2}{\partial C};\ \frac{\partial f_2}{\partial T}$$

all you need to do is you need to write equations corresponding to f_1 and the functions corresponding to f_1 and f_2 as functions of C and T. so r would be converted to $r = k_0 e^{-\frac{E}{RT}} C$ and then you do partial differentiation with respect to C and T; when you do this you can write a jacobian matrix. The jacobian would be

$$\underline{\underline{J}} = \begin{bmatrix} \frac{\partial f_1}{\partial C} & \frac{\partial f_1}{\partial T} \\ \frac{\partial f_2}{\partial C} & \frac{\partial f_2}{\partial T} \end{bmatrix}$$

And then you will determine this if you remember the procedure, you will determine these jacobian matrices at steady states, so steady state let me write it explicitly

$$\underline{\underline{J}}|_{T31},\quad \underline{\underline{J}}|_{T32},\quad \underline{\underline{J}}|_{T33}$$

This will be the first step. Then you will determine the eigen values. It is a two-by-two system so there would be two Eigen values; when you plug in all the values of say the heat transfer coefficient and density flow rates and so on, when you do this then you will realize that these three points which you obtain this point 1, point 2 and point 3 have different stabilities. So, you will find after doing this analysis that the middle point T_{32} is unstable, this point is stable and this point is also stable you will get this. Let me repeat what you are going to do; you will take function f_1 and function f_2, you will do the partial derivative, you will determine $\frac{\partial f_1}{\partial C}$, $\frac{\partial f_1}{\partial T}$, $\frac{\partial f_2}{\partial C}$, $\frac{\partial f_2}{\partial T}$, from where you will get the jacobian.

The jacobian will be determined at these three steady state temperatures; when you determine the jacobians, expressions for jacobians, in fact the components for the jacobian at these three points you will be in a position to determine the corresponding Eigen values. These eigen values will always be such that the middle point is unstable which means that both the eigen values would be positive that is the nature we saw previously and the first and the last points would be stable, which means that the eigen values would either both be negative or if they are complex numbers then the real part would be less than zero, the real part would be negative we saw that in both the cases the system is stable. One case would be sink solution the other case would be a spiral sink solution. So therefore, when I have this particular diagram in front of me let me draw this diagram again and do a further analysis.

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So, this is jacket temperature versus steady state temperature, the system looks like this so I have now this particular bound to my system and this portion will not be observed because this is you will do it for large number of different parameters and this portion is unstable, you take any of the vertical lines in this portion you will not get any stable solution. So therefore, you will not observe the system, so if you start your system vertically in this proximity, if you are away from this particular line, you will come to that line, come to that point.

Similarly, vertically if you start in the proximity of this point, you will end up at that point at the steady state, but I am now keeping on decreasing the temperature, my jacket temperature. If I keep on decreasing my jacket temperature what I see is that I no more am on that particular stable point, because now I am in this unstable region and I come down to this point.

Similarly, if I start from lower temperature and go, you end up here so this process of going up is called ignition because now you are not able to control your temperature the temperature is automatically going up because you are in the unstable region, so this process is called ignition and this process of coming down is called extinction.

So, you see an ignition-extinction behavior in case of this adiabatic operation and then this was a particular case when you took the x-axis or you did the analysis with jacket temperature, you can draw this curve for feed temperature as well. The nature of this curve would be same, hysteresis is what you would observe there as well. You can take this x-axis as the space space time again you will see a very similar behavior that you will see a hysteresis you will see ignition and extinction behavior in your system and then what you will see is that this seemingly very simple system which is a CSTR, you are stirring it, you are sending a jacket fluid and a very simple reaction A going to B, not reversible simply irreversible reaction, not very complex kinetics first order kinetics KCA gives to this exotic behavior in the dynamics of your system.

So what we saw today is that when you have non-linear dynamics, when you have a CSTR which is operating under diabetic condition you may experience dynamics which would be non intuitive, intuitively you may feel that if I start with one set of parameters of my system and I maintain a steady state then I should get a unique steady state temperature in my system that in fact may not happen I should not say does not happen that may in fact may not happen because your system is highly non-linear and what is the reason behind this observation of non unique steady states? The key reason behind this is that you have an energy removal curve in your system which is non-linear sorry not removal, generation curve you have a heat generation curve in your system which is non-linear.

Your heat removal curve was linear, your heat generation curve was non-linear, so there was a possibility of intersection of these two curves; one linear one non-linear at multiple points. In fact, if you remember our previous discussion, you have saddle node or tangent bifurcation in your system in which you can have the intersection at just one point, you can have intersection at two points and in this particular case you can have intersection at three points, and because you have multiple intersections, you have multiple steady states.

So now it is important to determine whether the steady states which you observed are stable or unstable? That can be done with the help of linearization, why are you assured that this linearization would work, if you go back to our theory, you will find that the solutions are hyperbolic, which means none of the Eigen values are actually zero.

So therefore, in certain cases you will get three eigen values, in one case both of the eigen values would be greater than zero, they would be positive so and that would happen for the middle steady state, your system would move away from that that would be the unstable steady state. The others true steady states would be stable they can be sink solutions, which means both the eigen values would be negative, they can be so spiral sink solutions which means that with oscillations you will settle down to that particular steady state solution. So, we will stop here today; we saw how interesting non-linear dynamics of reactors are, we will take two more examples of nonlinear dynamics in the week to come, till then good bye.