Advanced Process Dynamics

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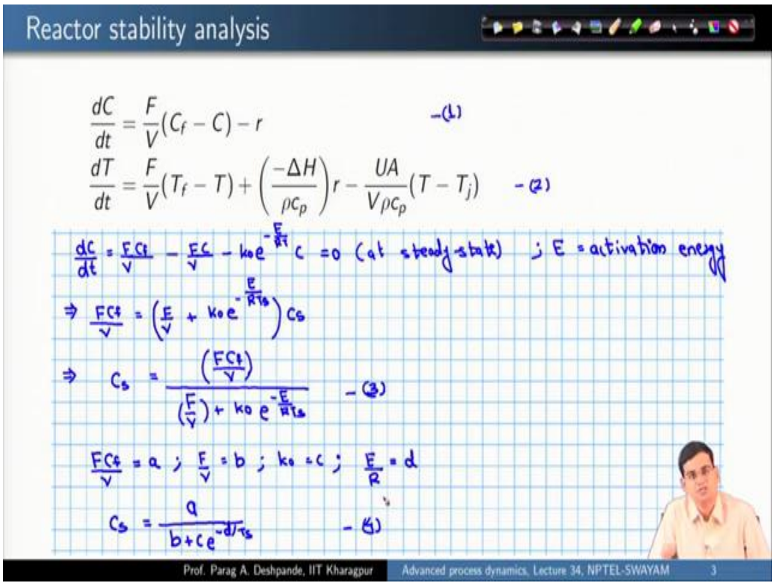
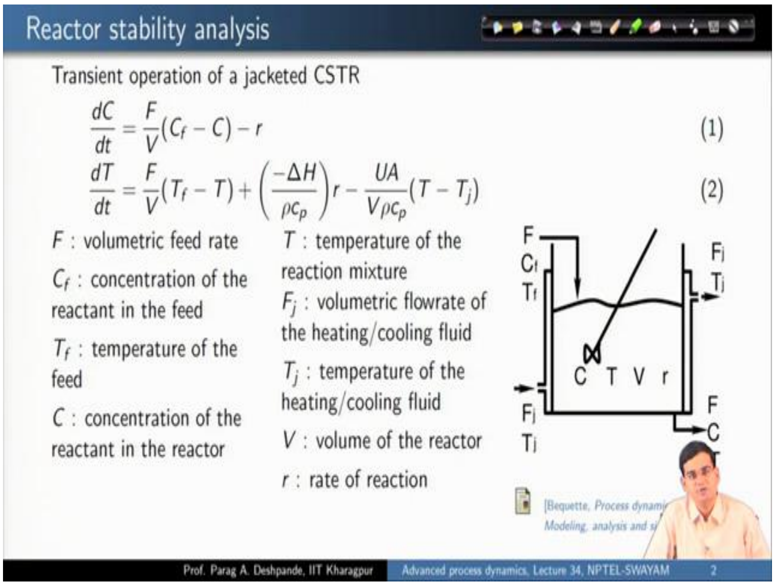
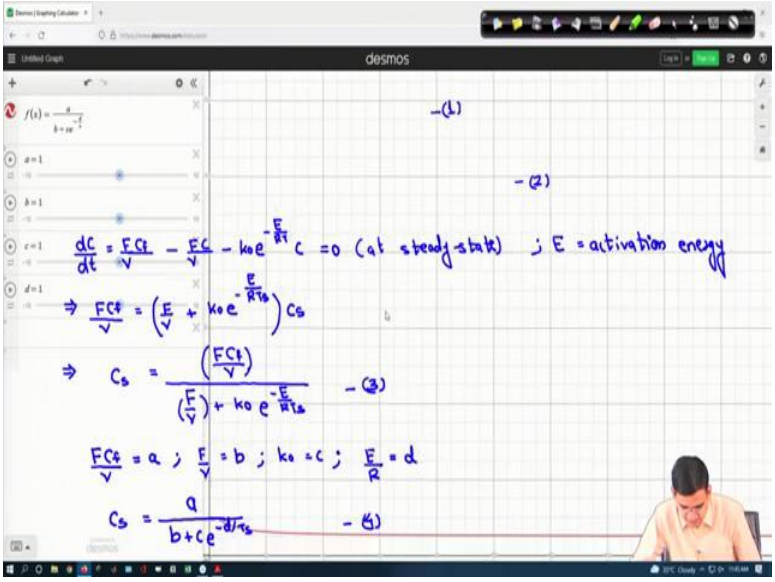
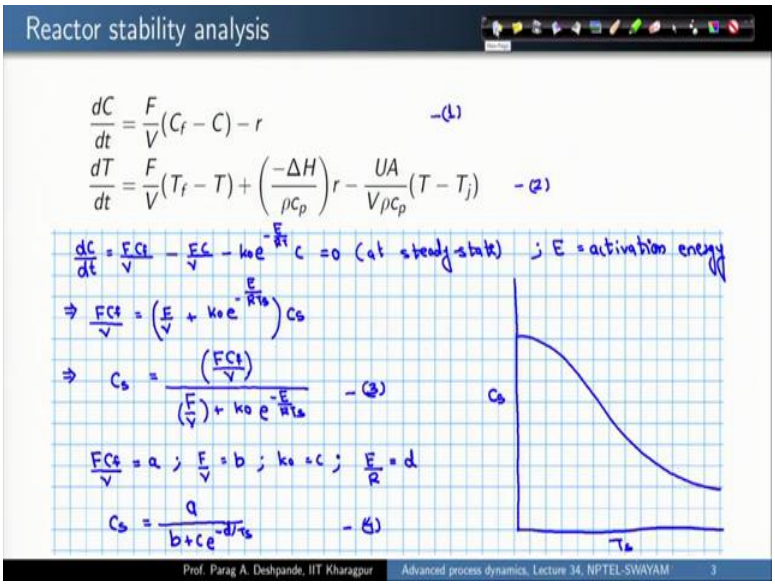
Lecture 34

Reactor Stability Analysis (Continued)






desmos
$f(x) = \frac{a}{b + ce^{-\frac{d}{x}}}$
a = 1
b = 1
c = 1
d = 1
-(1)
-(2)
$\frac{dC}{dt} = \frac{FC_f}{V} - \frac{FC}{V} - k_0 e^{-\frac{E}{RT}} C = 0$ (at steady state) ; E = activation energy
$\Rightarrow \frac{FC_f}{V} = \left(\frac{F}{V} + k_0 e^{-\frac{E}{RT_s}}\right) C_s$
$\Rightarrow C_s = \frac{\left(\frac{FC_f}{V}\right)}{\left(\frac{F}{V}\right) + k_0 e^{-\frac{E}{RT_s}}}$ -(3)
$\frac{FC_f}{V} = a$; $\frac{F}{V} = b$; $k_0 = c$; $\frac{E}{R} = d$
$C_s = \frac{a}{b + c e^{-d/T_s}}$ -(4)


Reactor stability analysis
$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r$ -(1)
$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right) r - \frac{UA}{V \rho c_p}(T - T_j)$ -(2)
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C_s
T_s
Prof. Parag A. Deshpande, IIT Kharagpur
Advanced process dynamics, Lecture 34, NPTEL-SWAYAM
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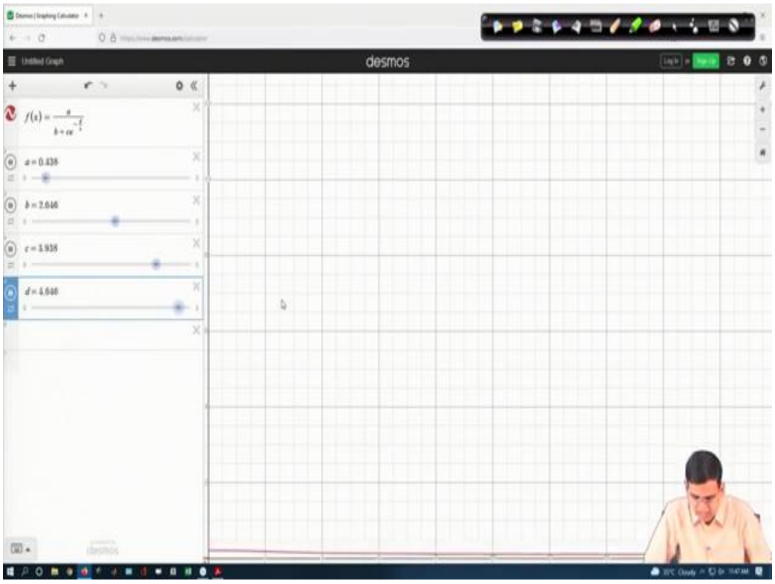
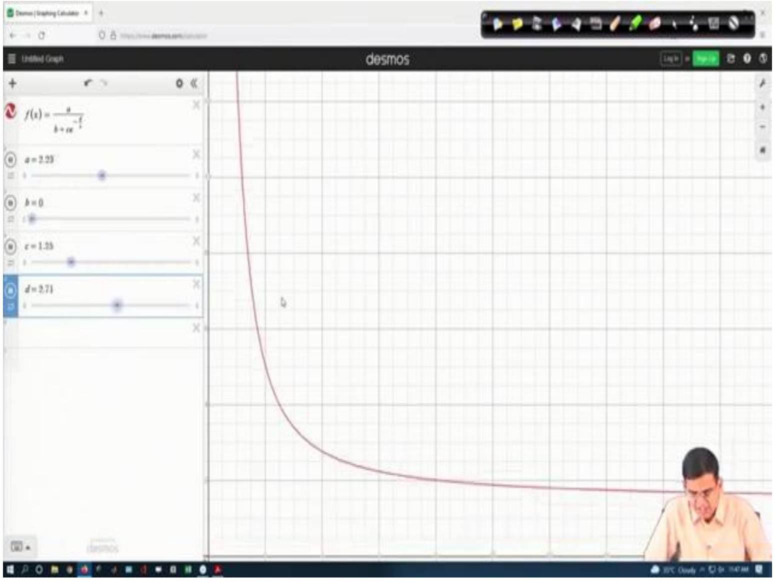
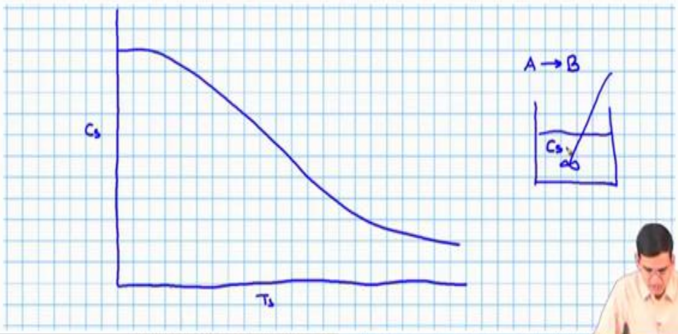

desmos
$f(x) = \frac{a}{b + ce^{-\frac{d}{x}}}$

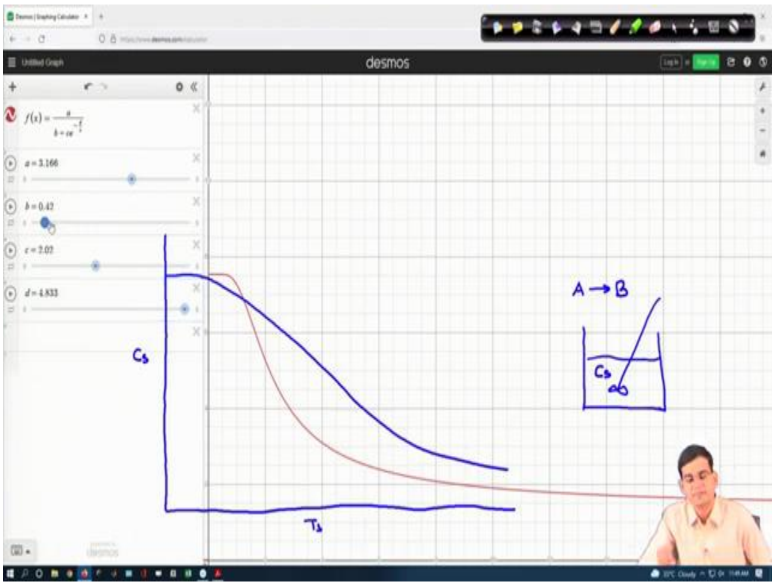


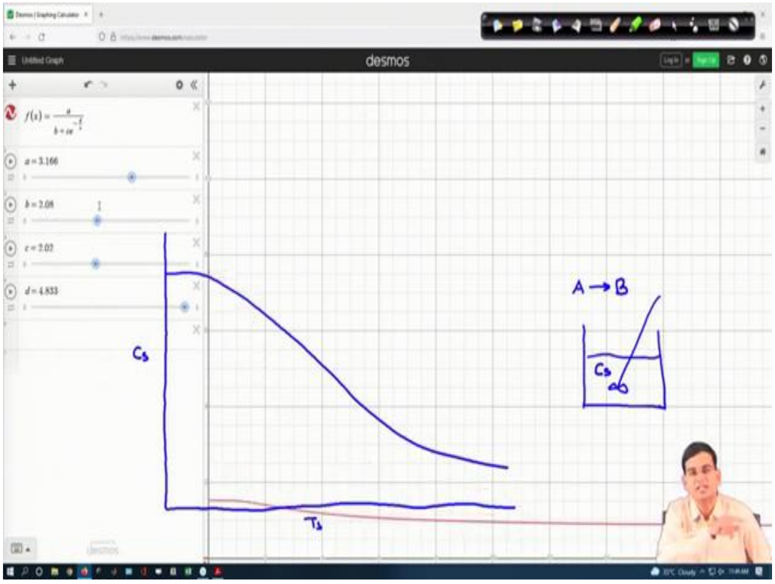
Reactor stability analysis

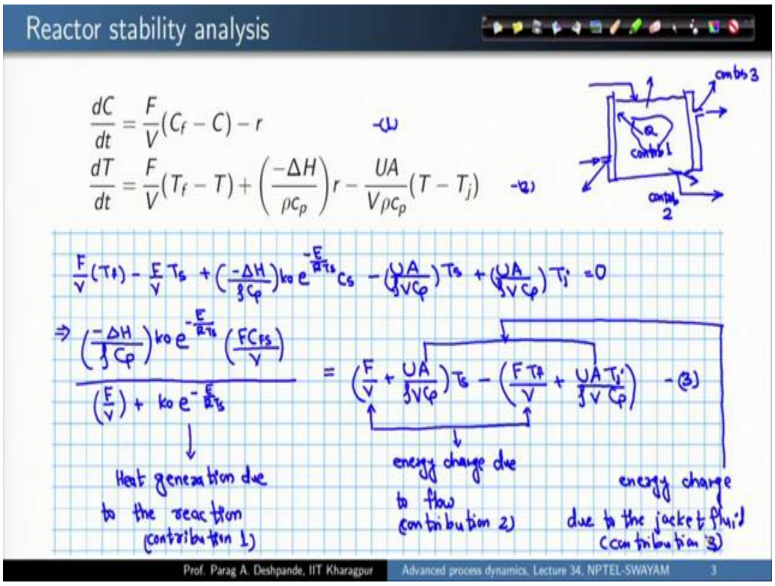
$$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r$$

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









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Let us continue our analysis of reactor stability, the system is in front of you just as a quick reminder; we were dealing with diabetic operation of jacketed CSTR that we actually analyzed the genesis of the two dynamical equations that are in front of you,

$$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r \dots\dots\dots (1)$$

$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right) r - \frac{UA}{V\rho c_p}(T - T_j) \dots\dots\dots (2)$$

What are the various assumptions, it is important that we absolutely know and remember the assumptions that were made during the analysis and we finally came to two equations which are of the form which is given in front of you. So, let us now analyze these equations, the first thing which you would like to do is to know the steady state.

So, looks like the first equation, so, let me refer this equation as equation (1) and this equation as equation (2). So, equation (1) is an equation which is explicit in C, there is no temperature term, so, in principle we should be able to solve this equation as a single equation, but that actually is not the case because the rate of reaction is a function of temperature. So, let us see what we can do here, so, I have

$$\frac{dC}{dt} = \frac{FC_f}{V} - \frac{F\text{C}}{V} - kC$$

We had assumed first order irreversible reaction and

$$k = k_0 e^{-\frac{E}{RT}}$$

k_0 pre-exponential factor.

$$\frac{dC}{dt} = \frac{FC_f}{V} - \frac{F\text{C}}{V} - k_0 e^{-\frac{E}{RT}}\, C$$

So, equation (1) itself has both concentration as well as temperature, but at steady state we know that this is going to be equal to zero.

$$\frac{dC}{dt} = \frac{FC_f}{V} - \frac{F\text{C}}{V} - k_0 e^{-\frac{E}{RT}}\, C = 0$$

So, assuming that I have a method to determine the steady state temperature which I do not at this point of time, but if I assume that I am somehow in a position to determine steady state temperature then its not very difficult for me to see that I can determine the steady state concentration as a function of steady state temperature. So, let us see how we can do that; I can write this as

$$\frac{FC_f}{V} = \left(\frac{F}{V} + k_0 e^{-\frac{E}{RT_s}}\right) C_s$$

So, I have used subscript s in concentration and temperature to indicate that this is a steady state condition and if that is the case then I can write C_s, the steady state concentration.

$$C_s = \frac{\frac{FC_f}{V}}{\left(\frac{F}{V} + k_0 e^{-\frac{E}{RT_s}}\right)} \ldots\ldots\ldots(3)$$

E is the activation energy.

So, we forgot this it has to be Ts, so, now if I know the steady state temperature then I can plug in the value of steady state temperature here in equation number (3) and I can determine the steady state concentration inside the reactor. I will come to that point that how to determine the steady state temperature, but before that let us see if we can know the variation of steady state concentration inside the reactor as a function of steady state temperature and by the way when I write this I have assumed that rest all the quantities also are at steady state which means that the invert flow rate is at steady state, the volume has been attained as constant, the concentration of the reactant in the feed is a steady state it is a constant value and So, on.

To analyze the qualitative behavior what I can do is I can set

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

If this is the case then I can write Cs as

$$C_s = \frac{a}{\left(b + \mathrm{c}e^{-\frac{d}{T_s}}\right)} \ldots\ldots\ldots(4)$$

and if I plot C_s as a function of T_s......... using this I can simply get the variation.

Before that I must know the nature of a, b, c, d......... volumetric flow rate is a positive quantity, concentration the feed is a positive quantity, volume is a positive quantity, so, a is positive. Similarly, $\frac{F}{V}$ will be positive, pre-exponential factor for a reaction is always positive, activation energy is always positive, R is a positive constant, so, therefore a, b, c, d..... all are positive constants.

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So, once I know this let me go to my desmos calculator and try to punch in this expression, so,

$$f(x) = \frac{a}{\left(b + ce^{-\frac{d}{x}}\right)}$$

Now the x-axis here is temperature always positive, y-axis is concentration always positive, so, I need to worry only about this quadrant. So, the general nature which I can draw here, let me draw it, I will analyze the dynamics further but this is steady state concentration, steady state temperature and what I see as a general trend is this, so, it would look something like this. Now let me try to find out various cases under which I may, if I have changes in the nature, so, I have 0 to 5. I am using these values to find out all the possibilities what you ideally should do is go back and try to determine say the heat transfer coefficient and the volumetric flow rate, the volume, rate constants and so on and punch in those values.

Here we are trying to understand the qualitative behavior So, therefore I am just setting these values like this, so, 0 to 5 and let me start animating to see the effect of all the parameters and in all the cases what I see is that the general behavior of my system conforms to this decrease in the steady state concentration with an increase in temperature. So, I can see how the variation take takes place.

So, let me stop the animation here and therefore what I see is a general nature of the curve which looks like this; C_s, T_s and does this make sense physically? Well, it does because if you have higher temperature there would be higher rate of reaction and since C is the concentration of the reactant for the reaction A going to B, more of A would be consumed at higher temperatures and therefore inside the reactor you have C_s would go down as the temperature increases and this is precisely what you can see here.

Now what you can also see here is that the moment I change this one of these quantities, so, b in our case for example was the ratio $\frac{F}{V}$and what happens to this ratio $\frac{F}{V}$, see here at lower $\frac{F}{V}$, you had a sharper decrease and at very large $\frac{F}{V}$, the decrease was not as sharp. Why does this happen, because you have now provided the system with an increase of $\frac{F}{V}$, the space velocity is very small and for very large and space time is very small. So, if the space time is very small you are not giving sufficient time for the reaction to take place and therefore there is not a large dip in the concentration inside the reactor, and the concentration then becomes constant even if you provide the system with large temperature.

Therefore, this analysis which we got by separating or taking explicitly that concentration equation assuming that there is some way to determine the steady state temperature looks to be correct. Now the problem is that we need to know the steady state temperature profile; if you know the steady state temperature you can plug it in the previous expression that we got and you can determine the steady state concentration. Now let us see how to determine steady state temperature.

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So, the steady state temperature can be determined by setting equation (2) to be zero. That is the definition of steady state anyway, so, what I can write here is this

$$\frac{FT_f}{V} - \frac{FT_s}{V} + \left(\frac{-\Delta H}{\rho c_p}\right) k_0 e^{-\frac{E}{RT_s}} C_s - \left(\frac{UA}{V\rho c_p}\right) T_s + \left(\frac{UA}{V\rho c_p}\right) T_j = 0$$

Again, it is important to realize that the flow rates here have been assumed to be at steady state which means they are constants, the jacket temperature T_j has assumed to be at steady state which means it's been assumed to be constant and concentration is already C_s which means it has been assumed to at steady state.

So, let me do some rearrangements here, let me write this as

$$\frac{\left(\frac{-\Delta H}{\rho c_p}\right) k_0 e^{-\frac{E}{RT_s}} \left(\frac{FC_{fs}}{V}\right)}{\frac{F}{V} + k_0 e^{-\frac{E}{RT_s}}} = \left(\frac{F}{V} + \frac{UA}{V\rho c_p}\right) - \left(\frac{FT_f}{V} + \frac{UAT_j}{V\rho c_p}\right) \dots\dots\dots (3)$$

Let me call this as equation (3) and equation (3)...... this rearranged form is a very important equation because it lets me make certain very important observations.

So, let us see and why did I do this particular rearrangement, so, if I remember the genesis of the energy balance equation then I have a vessel with a jacket and there is an inflow, there is an outflow, you maintain some constant volume and there is an inflow and outflow of the jacket fluid.

So, if I analyze this process of reaction and energy transfer then what I see is that I have the generation of heat because of the reaction, let us assume the case where the reaction is exothermic. So, therefore I have generation of heat because of the reaction, so, let us say that heat is being generated by the reaction. Now what is the meaning of the term that I have a steady state? I have a steady state means that there are no gradients in time that means the temperature is no more changing in time.

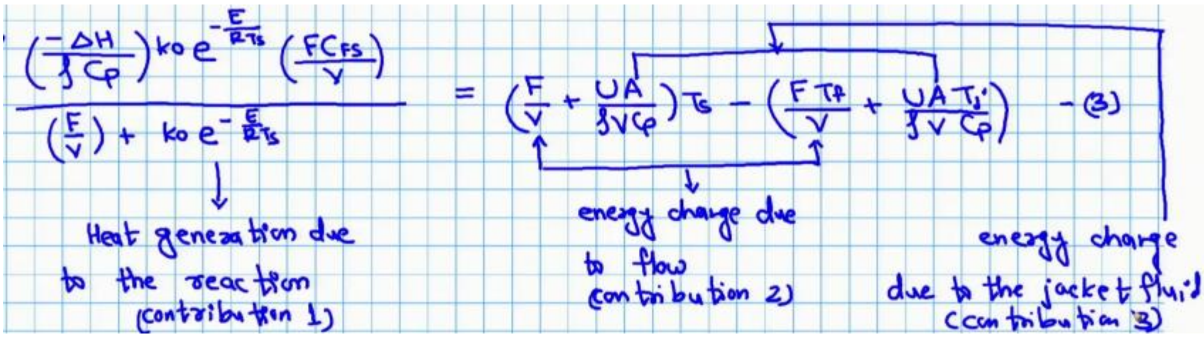
Now if I am generating heat because of my reaction the temperature of my reaction mixture must increase, but since I am observing that I am at steady state and there is no change in the temperature of my system then there must be something in my system which is taking my heat away.

So, equation (3) which you can see here has three components, the one on the left hand side involves ΔH which is the heat of reaction and it involves the rate of reaction, so, this entire term on the left hand side is a term which gives you the heat generation due to the reaction and this must be carried away from the system for the system to have constant temperature which means for the system to be at steady state. So, what are the two mechanisms where this is this is happening well it is happening because some of the material is coming in and some of the material is going out.

So, this process of inflow and outflow is taking some of the energy away and which is that term which would represent this; well this particular component and this particular component these two would be responsible for energy change due to the flow in the system, material is flowing in and flowing out and it is carrying energy and therefore if the energy is being generated, it is possible that more energy is being taken out by the outlet stream than what is being supplied by the inlet stream, it is one of the possibilities, so, this is one factor.

Another factor is this; so, this factor which means that the energy changes due to the jacket fluid and that is the whole point of having the jacket anyway; that if you are at a large temperature, you send a cold fluid through the jacket then the fluid in the jacket will get heated up, it would receive energy and then that would be energy which is being generated by the reaction.

So, I will have an energy change across this, so let me write this as contribution 1, so, this is contribution 1. This if I write as contribution 2, if this is written as contribution 2, so then this would be contribution 2. So, let me change the direction of arrow a little bit outward arrow means the direction of energy change and then I will have contribution 3 and let me write this as 3.



So, when I write this entire energy balance and rearrange this in this manner what I see is that I have the energy balance or rather the attainment of steady state because of the mere fact that if I am at steady state the heat generated by the reaction must be compensated or must be carried out of the system, either because of the inflow or because of the outflow of the material of the reaction mixture or because of the jacket fluid. This is the genesis of the rearrangement of this equation.

Now how can I possibly make use of this equation to determine the steady state temperature? Well, what I see here is that I have a function on the right-hand side which involves $\frac{F}{V}$, which involves the heat transfer coefficient, which involve it involves the temperature of the jacket fluid, and so, on and what I also see is that I have an expression on the left-hand side which involves the heat of reaction, which involves the pre-exponential factor, which involves the activation energy and so, on.

If these two expressions have to be equal, if a steady state has to be attained then at steady state these two expressions will become equal, the left-hand side in other words the intersection of left-hand side and the intersection of the right-hand side will be satisfied by a condition, which is given as the steady state temperature. So, one of the strategies to solve this equation would be to plot the left-hand side and to plot the right-hand side individually and the intersection of the left-hand side function and the right-hand side function will give me the steady state temperature.

Now if I need to determine the steady state temperature; steady state temperature would correspond to, as I made a mention before that I have assumed that the inlet flow rate is constant, your feed concentration is a constant, flow rate of the jacket fluid is constant, temperature of the jacket fluid everything is constant everything is steady state, so, therefore if I take up a particular set of values of different parameters, I fix the flow rate of the fluid of the reaction fluid, I fix the flow rate of the jacket fluid, I fix the temperature of the jacket fluid, I fix the concentration and temperatures of the reaction mixture, I fix all of them then I will throw in all of these values in the left hand side, the only variable which I will be left with would be Ts steady state temperature. So, I will draw the left-hand side as a function of Ts.

Similarly, I will determine the heat transfer coefficient, heat transfer area and so, on. I will plug them on the right-hand side, I will draw that curve and the intersection should give me for that particular state of that particular set of variables the steady state temperature. Now what but you see here in this particular case especially in the left-hand side is that the system is non-linear, you have an exponential function. So, is there a guarantee that if I have a set of parameters corresponding to the steady state of your system will I get a unique steady state temperature? Since the system is non-linear, I cannot guarantee, I cannot say it for sure at least just by looking at these equations. So, how many solutions would exist, what would be the nature of the solutions, what would be the stability of the solutions, all of these need to be analyzed, we will do this in the next lecture, till then good bye.