Advanced Process Dynamics

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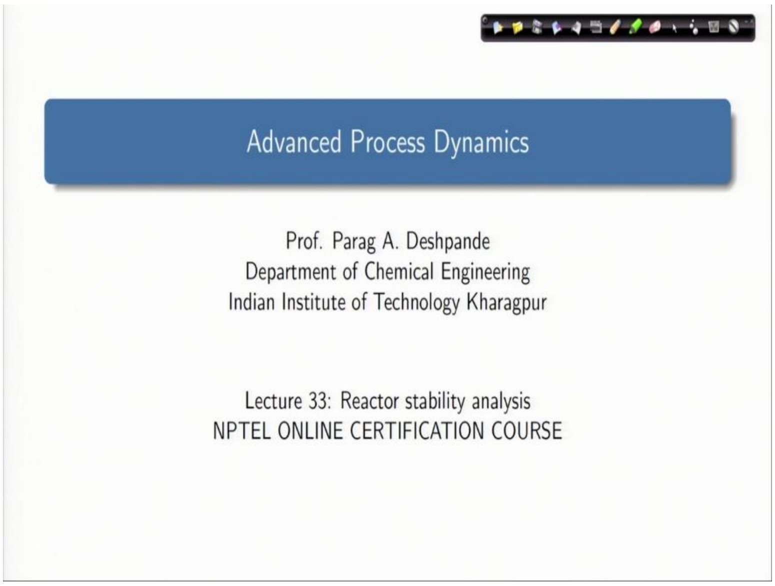
Lecture 33

Reactor stability analysis



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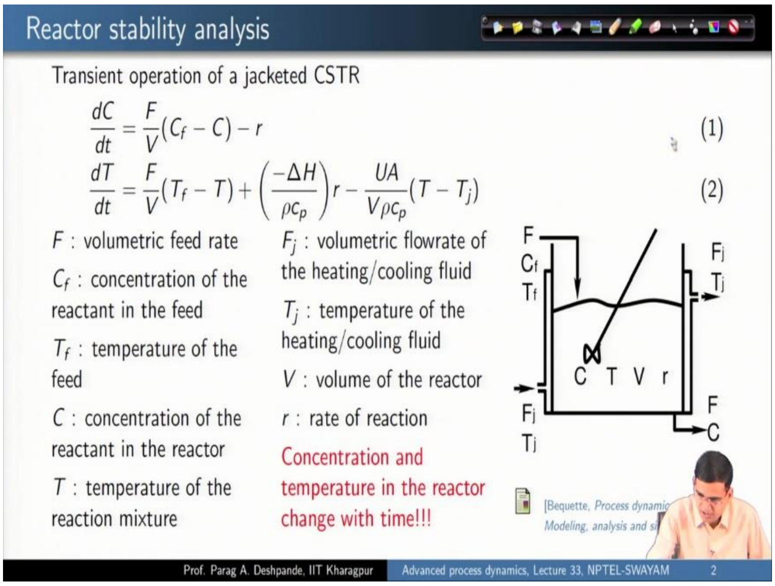
Lecture 33: Reactor stability analysis
NPTEL ONLINE CERTIFICATION COURSE



Reactor stability analysis

Transient operation of a jacketed CSTR

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

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

F : volumetric feed rate

C_f : concentration of the reactant in the feed

T_f : temperature of the feed

C : concentration of the reactant in the reactor

T : temperature of the reaction mixture

F_j : volumetric flowrate of the heating/cooling fluid

T_j : temperature of the heating/cooling fluid

V : volume of the reactor

r : rate of reaction

Concentration and temperature in the reactor change with time!!!

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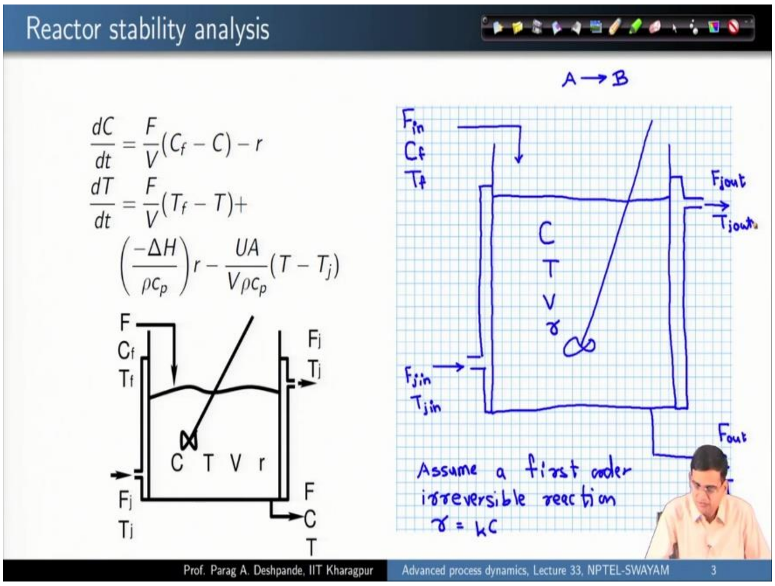


Reactor stability analysis

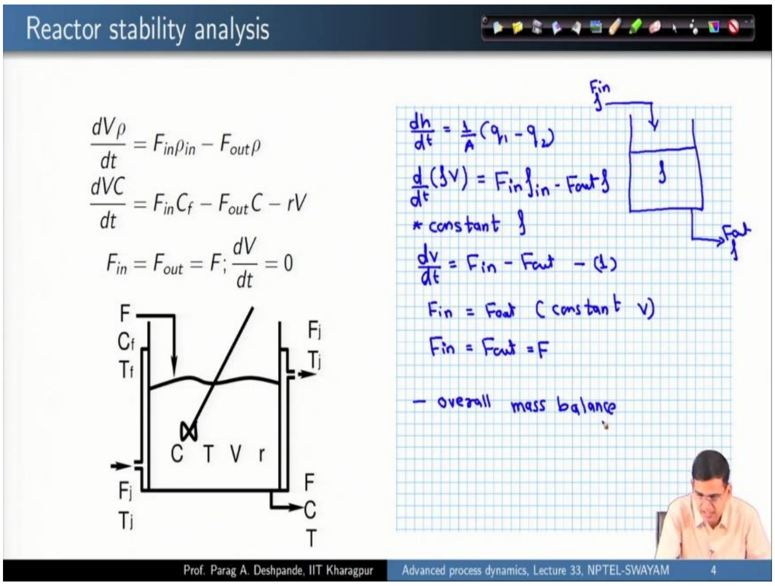
$$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r$$

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

$A \rightarrow B$

Assume a first order irreversible reaction

$r = kC$



Reactor stability analysis

$$\frac{dV\rho}{dt} = F_{in}\rho_{in} - F_{out}\rho$$

$$\frac{dVC}{dt} = F_{in}C_f - F_{out}C - rV$$

$$F_{in} = F_{out} = F; \frac{dV}{dt} = 0$$

$\frac{dh}{dt} = \frac{1}{A}(q_1 - q_2)$

$\frac{d}{dt}(\rho V) = F_{in}\rho_{in} - F_{out}\rho$

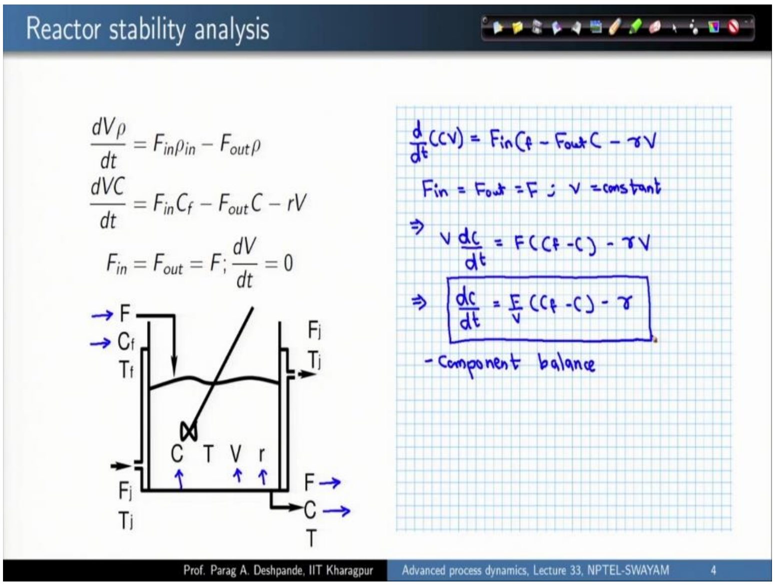
* constant ρ

$\frac{dV}{dt} = F_{in} - F_{out}$ – (1)

$F_{in} = F_{out}$ (constant V)

$F_{in} = F_{out} = F$

– overall mass balance



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$$F_{in} = F_{out} = F; \frac{dV}{dt} = 0$$

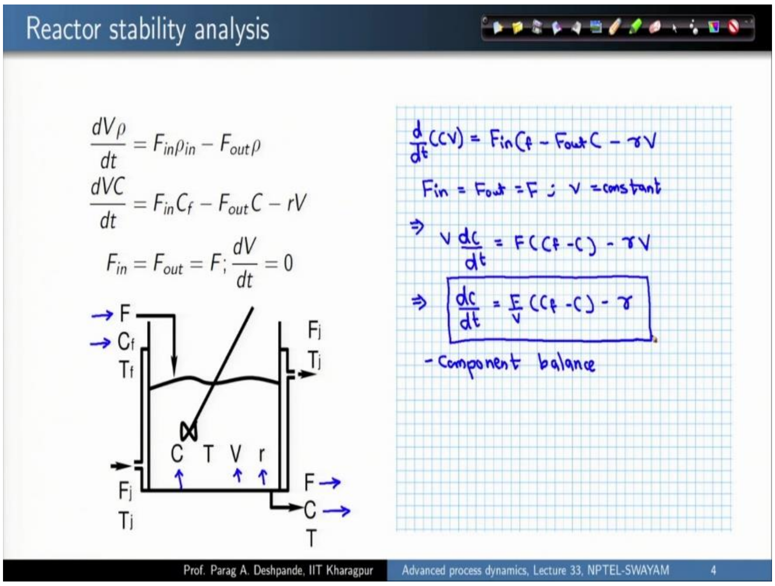
$\frac{d}{dt}(CV) = F_{in}C_f - F_{out}C - rV$

$F_{in} = F_{out} = F$; V = constant

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

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

- Component balance



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

- Component balance

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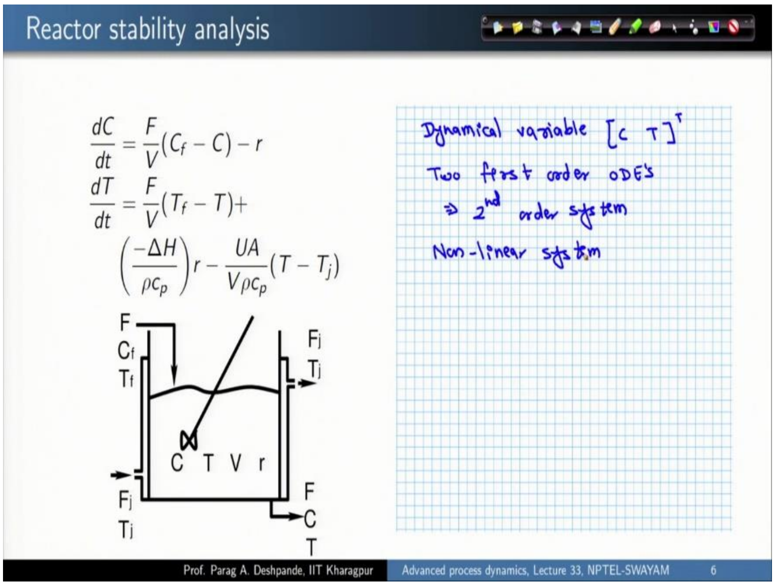

Reactor stability analysis

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

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

Dynamical variable $[C \quad T]^T$

Two first order ODE's

$\Rightarrow$ 2^{nd} order system

Non-linear system

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So, we continue our discussion on nonlinear dynamics. And in the previous lecture, we had a look into the theory of higher order dynamical systems. So, now, what we will do is for the next few days, we would be focusing on various applications, where we would see how the theory developed rather studied by as for nonlinear dynamical systems of higher order can be used for the analysis of systems which are of relevance to process engineering as well as to the natural sciences. So, today we will take one particular example of reactor stability analysis.

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So, let us have a look into the system that we have in front of us, we had this example, right in the first lecture, where we saw that we have the case of transient operation of a jacketed CSTR. CSTR stands for continuous stirred tank reactor. We gave two model equations

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

and

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

Various quantities have been elaborated below.

And we saw that this is a dynamical system because the concentration of species inside the reactor changes with time when you are doing a transient operation and so, does the temperature of the reactor. We would see today that there are various forcing functions which act upon the system the flow rate of the reactants for example, is a forcing function the temperature of the jacket can act as a forcing function and so on. So, we will see how does the dynamics of the system behave in this particular case, when we can see that this particular set of equations in fact, nonlinear equations when we plug in the rate expression in this particular equation, then we will see that the system is highly nonlinear and then we will try to understand the dynamics, especially the dynamics around the steady state.

So, before we go into the details, let us first try to understand what the system is really about, what are the various assumptions under which these particular equations would remain true? And what are the assumptions and approximations under which we can do the dynamical analysis. And if that were the case, the dynamical analysis would be true for certain ranges of the parameters of the system and what are those ranges under which we can expect the analysis to hold true.

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So, let us have a look into this particular system. So, what we have is a CSTR. So, it is a tank which is equipped with a stirrer. So, that it is assumed that there is a complete mixing of the contents inside the reactor, it is a continuous mode of operation. So, there would be an inlet flow. So, let us say that the flow of material in comes at a volumetric flow rate F in. So, F in is the volumetric flow rate of the material which is coming in. In the inlet, the concentration of the species is maintained as C_f, f stands for feed, so, the concentration of the species in the feed and then what will also be there is that there would be a corresponding temperature of the inlet stream and that would be denoted as T_f.

The material would also be continuously flowing out so, I have an outlet stream and before I can write anything about outlet stream, let me first try to understand what goes on inside the reactor. So, the material flows in with certain concentration of the species and let us say that an irreversible reaction A going to B takes place inside the reactor, we have assumed that the reaction is irreversible and we are tracing only the concentration of A if the temporal profile of concentration of A, then you would automatically know the temporal variation of B using the simple reaction equation.

So, see everywhere in our notation simply refers to the concentration of the species. So, now, once the species enters in the reactor, the reaction takes place and that well mixed contents have the concentration C. So, concentration of A inside the reactor is simply denoted by C. There are no special variations inside the reactor this is an assumption that there are no special variations inside the reactor and since there are no special variations in concentration, the system is well mixed you can as well as the room that there is a constant temperature T inside the reactor and since the contents of the reactor are simply flowing out from the outlet stream, you can say that the contents here at the outlet also have the concentration C they are at temperature T but the flow rate may be different at this point of time we may not say anything about the flow rate, so, therefore, the volumetric flow rate is F_{out}.

Now inside the reactor the reaction mixture will have some volume and let us denote that volume by V and the intrinsic reaction rate for this system is denoted by r. Now, if we assume so, if we assume a first order irreversible reaction taking place inside the reactor then I can write

$$r = kC$$

I have not used the subscript A because we are following only the concentration of A. So, kC_A or kC in this particular case is the expression for rate of reaction.

Now, having known this I have now analyzed what is going on as a flow process and as a reaction in the reactor. Now, what you can have is, a situation where the reaction is exothermic meaning that some amount of energy would be liberated heat would be liberated by the system and if you want to maintain a constant temperature T, then you will have to take that heat out of the system. So, therefore, this particular arrangement is also called diabetic operation of the reactor diabetic operation of reactor means that actually in your feed is allowed in the system.

So, what can be a possible arrangement in which you would be in a position to take out the heat from the system? I will put a jacket around my reactor. So, let us say that I have a jacket and there would be a stream of the cooling fluid which would be going continuously in and it would be coming continuously out. So, again the volumetric flow rate of the cooling fluid can be denoted as F_{jin} volumetric flow rate of the jacket fluid or the cooling fluid, inlet and F_{jout} and temperature T can be denoted as T_{jin}, the temperature jacket fluid at the inlet and T_{jout} is the temperature of the jacket fluid at the outlet....... nothing more than this specification is required.

Now, this is the most general synthesis of the process the adiabatic transient operation of a CSTR which has been presented in front of you. To obtain the model equations which have been shown on the left-hand side and certain quantities which are different from what has been drawn on the right-hand side, then what has been shown on the left-hand side... we need to carefully look at the assumptions. So, the overall picture is this that what you can see on the right-hand side is that there is an irreversible first order reaction A going to B which is taking place in a CSTR, the inlet flow rate is F_{in} volumetric flow rate, the concentration of the species A is in the feed C_f, it comes at temperature the T_f.......... f stands for feed.

There is a well mixed system inside the react, so, there are no temperature or concentration gradients, spatial gradients inside the reactor. So, therefore, concentration of A inside the reactor is C, temperature is T, the volume is V. At this point of time, we do not know of we cannot say whether the volume V of the reaction mixture is constant or variable we are just denoted as V, the rate of reaction is r and then since, this is the case that you are very well mixed case at the outlet, you have the concentration of the species is simply C which is same as that in the inside the reactor and temperature T which is same as that inside the reactor.

The volumetric flow rate would be F_{out} at this point of time we do not know the relationship or inequality which exists between F_{in} and F_{out}. Similarly, to maintain a constant temperature to take out the heat of reaction for the case of exothermic reaction to supply also equivalently the heat to the system for an endothermic reaction, you generally will not have a jacketed system, you will have a coil system, but in either case to have the energy exchange for a diabetic operation, you have the flow rate of the fluid in the jacket given as F_{jin} and outward flow rate outlet flow rate as F_{jout}.........j stands for jacket.

Similarly, your temperature at the inlet as T_{jin} and temperature at the outlet as T_{jout}. This is the entire description of the system. Now, we will make certain approximations, we will make certain assumptions to reduce all of these quantities which have been shown on the right-hand side to conform to the equations which have been given in the left-hand side.

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So, let us see what those approximations are. So, the first thing which I can do is I can write a mass balance over the system. So, I have simply a tank. So, this is my tank in which material is coming in, material is going out certain level is maintained. This is the classic example of liquid level system which we have been studying right from the first day. Remember our equation that there used to be

$$\frac{dh}{\mathrm{dt}} = \frac{1}{A}(q_1 - q_2)$$

That used to be a mass balance equation with q_1 as the inlet flow rate and q_2 as the outlet flow rate.

So, for the overall mass balance, it is the same case you have the rate of change of mass inside the system given as

$$\frac{d}{\mathrm{dt}}(V\rho) = F_{in}\rho_{in} - F_{out}\,\rho$$

Remember, when we solved this particular case, previously, we had assumed constant density and density got cancelled out from both the sides. Now, we are explicitly taking the density in this case and this would be equal to what if there occurs achieved in the density of the system.

If there occurs a change in the density of the system, which means that the density in the inlet is something different and density at the outlet is something different.

Now, under an approximation that you have constant density the density does not change well anyway you would not expect a temporal change in the density of the system, but there may be temporal variation in the temperature of the system and with changes in the temperature of the system the density may change and that is how temporal variation of the density may happen as well as spatial variation may happen, when you compare the density at the inlet and density at outlet.

When you assume that this does not happen, which means that you have a constant density that then under such a case I can simply write

$$\frac{dV}{\mathrm{dt}} = F_{in} - F_{out} \ \dots\dots\dots (1)$$

So, the first thing you will see that in your original equations there were no densities and now, you see that we have gotten rid of density because we have assumed that the density does not change this is an approximation and we must remember that we have made this approximation so, subsequent analysis would be true as long as this approximation holds true.

Now, we have this first equation, which is

$$\frac{dV}{\mathrm{dt}} = F_{in} - F_{out}$$

Now, imagine that you do an operation in which you will maintain the liquid level. So, under such assumption the volume the overall reaction volume, the volume of the reaction mixture remains constant. So, you have inlet flow rate, you have outlet flow rate and the liquid level in the tank in the CSTR remains constant........ which means the volume of the reaction mixture remains constant......... in which case I can write

$$F_{in} = F_{out} \qquad (constant\ V)$$

which means constant volume and when $F_{in} = F_{out}$ which means, the total mass which is coming in is equal to the total mass which is going out then under that condition I can simply write

$$F_{in} = F_{out} = F$$

and that is the F which you see in the diagram on the left-hand side the volumetric flow rate you are assuming that the operation is taking place at a steady state.

So, there is no change in the volume of the system and therefore, the inlet flow rate is equal to the outlet flow rate. So, this was the overall mass balance, what now, we can do further is do a component balance. So, this was the overall mass balance it is the result of overall mass balance that we got an idea that the inlet flow rate would be equal to the outlet flow rate. So, therefore, we have changed F_{in} and F_{out} to simply one quantity F which is the volumetric flow rate of the quantities which are flowing through the system.

Now, we can do a component balance how does the variation of the reactants or the products take place in the system, we will do only one because the other one can be obtained pretty trivially.

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So, now I can do the component balance, if C is the concentration, so, then the amount of A inside the reactor this temporal variation would be given by

$$\frac{d}{\mathrm{dt}}(VC) = F_{in}C_f - F_{out}\,C - rV$$

Now, some of the A would be coming in inside the reactor they would be reaction and the unreacted A would flow out. So, I have three processes going on, change in the concentration because from the inlet stream A is coming in, change in the concentration because from the outlet stream A is going out and within the reactor changes taking place anyway because of the reaction.

So, r is the rate of reaction, which is which would be expressed per unit volume. So, when you multiply it with volume, you will get the time rate of change of the concentration of A in the reactor because of the reaction.

Now, we have assumed that

$$F_{in} = F_{out} = F$$

and therefore, from here and volume is constant. So, I can write this as

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

in other words

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

This is the equation which we get from component balance so, by looking at the figure which is on the left-hand side, now I mean in a position to appreciate that why I have F here and F here..... instead of F_{in} and F_{out}, ... why I have C_f and I cannot say anything about T_f . Just by the mass balance. So, let me not put any arrow here. I have why I have C here which is the same C here and why I have a V here and why I have a have an r here.

So, using mass balance and using component balance, I could get this particular equation which is our working dynamical equation one of the working dynamical equations. The second dynamical equation involved temperature and to have an idea about temperature we need to do energy balance. So, let us look into the energy balance.

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So, now, I have a system in which I have the variation of temperature a possible variation of temperature and heat exchange is allowed. It is a diabetic process. So, therefore, mC_PT. if mC_PT is the energy content of your system. Then, I can write

$$\frac{d}{\mathrm{dt}}\left(V\rho c_p T\right) = F_{in}\rho_{in}c_pT_f - F_{out}\,\rho c_p T + (-\Delta H)rV - UA(T - T_j)$$

There would occur an energy change in the system because of the reaction, the reaction can be either endothermic or exothermic. So, if the reaction is exothermic energy will be added to the system, the reaction is endothermic the energy would be extracted by the system and therefore, depending upon that you will have either positive or negative sign for ΔH. So, $(-\Delta H)rV$, where r is the rate of reaction. So, this is the energy change because of the reaction.

Now, you have a jacket and across the jacket you have the energy change. So, therefore, this is given as $-UA(T - T_j)$. Now, this is an important assumption which we need to remember. So, now, what you have is a system in which the jacket has well mixed contents. So, the jacket is well mixed which means that there would not be any gradients, spatial gradients within the jacket. In other words, I can write

$$T_{jin} = T_{jout} = T_j$$

Let me say it again that the contents of the jacket have been assumed to be perfectly mixed, which means that there would not be any spatial gradients of temperature of the jacket fluid inside the jacket and therefore, $T_{jin} = T_{jout} = T_j$. What else do you assume? You have assumed constant density. So,

$$\rho_{in} = \rho = constant$$

This you have established in the previous balance V is a constant and now, what you are also assuming is that the material properties a constant which means that specific heat we know that specific heat can be a function of temperature, but for this analysis we have assumed that c_p is a constant and also

$$F_{in} = F_{out} = F$$

If this is the case, then you simply write this as

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

This becomes your balance equation. So, this is the energy balance. Now certain assumptions further in this case are observations rather you have $-UA(T - T_j)$. This basically means that you have the flow of heat from the system from the reaction mixture to the jacket fluid.

So, which in turn means that you must be having an exothermic reaction and if the reaction is exothermic then you see that the term which involves the energy contribution or energy change from the reaction has a $-\Delta H$, which means that you have the energy addition because of the generation of energy because of the reaction and that energy is taken away by the jacket fluid. So, these are the again observations which you should make for this particular equation.

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So, by the overall mass balance component balance and the energy balance you can see that these are the two equations which you have in front of you and these are your dynamical equations. So, your dynamical variable in the present case will become...... $[C \quad T]^T$. C, the concentration of A inside the reactor and T, the temperature of the reaction mixture in the reactor. You have two equations both are first order. So, I have two first order ODE's which means I have a second order system.

Now, everything which we studied about second order dynamics should now come in front of you that what all can happen to this particular system. Further one more thing which you can write about this is that this is a non-linear system. So, if possible, you could solve this nonlinear system directly and get the temporal variation of concentration and temperature with time. If not, then you will tend to linearize the system and analyze the linear dynamics.

In other words, you will determine the steady state, concentration and temperature in the system, about the steady state you will analyze the dynamics of the system by doing the linearization of the equations which we developed. So, what we will do is we will stop here today. And in the next lecture, we will continue this discussion and try to understand the dynamical features as well as the steady state features of the system. Thank you.