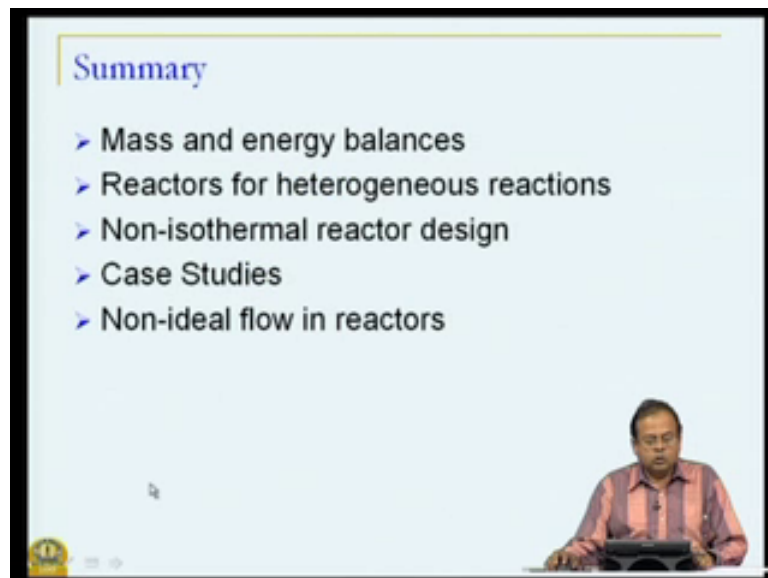


**Chemical Reaction Engineering**  
**Prof. Jayant Modak**  
**Department of Chemical Engineering**  
**Indian Institute of Science, Bangalore**

**Lecture No. #40**  
**Problem solving: Reactor Design**

Friends, this is our last session of this course and today we will be solving some problems in Reactor Design. Now, if you **if you if you** recall or you can always of course, go back to your video lectures and recall, if you do not remember. In the last module namely the reactor **reactor** design, we discussed several aspects, so let us quickly summarize those and then look at few problems.

(Refer Slide Time: 00:53)



So, what we started out was essentially looking at mass and energy balances for reactors in general, both tubular or fixed bed reactors, tubular reactors in which plug flow or small deviation of plug flow, that kind of flow is occurring or a stirred tank reactor. And for stirred tank reactor, we wrote a general mass balance, so that, we can emulate batch process, continuous process or a semi-batch process using the same set of mass and energy balances only appropriately changing the feed rates; where for batch reactor there

is no feed in and out for semi-batch there is only feed in, but no feed out and for continuous reactor there are both feed in as well as feed out.

We then spent little bit of time, for writing the mass balance as well as energy balance for heterogeneous reactions. We talked mainly about gas solid catalytic reactions here, so here the idea is firstly we recognize that, not entire volume or the void volume of the reactor is available, for the transport in the bulk. So, if we write the mass balances for reactants and products in the bulk; all that bulk is experiencing is of course, the convective transport and disappearance from the bulk due to diffusion into the catalyst.

So, we wrote a very generalized scheme by writing a mass balance, such that we say that, there is some flux or there is some rate at, which material is disappearing. And based on this, we had different types of models for example, if you say that diffusion limitations are not there, then the disappearance rate or rate of those disappearance processes, is same as the reaction rate. Therefore, what we had a pseudo homogeneous model; **model** is very similar to homogeneous model that is, empty reactor models except, there is a wide fraction term which appears, so pseudo homogeneous model. But if you say that, transport in the catalyst is also important, then we had this disappearance rate equal to, that external mass transfer rate; because that is what only the gas phase will experience; it sending out material from the bulk to the reactor with the catalyst surface or receiving it, if it is a product.

But then, what happens to this disappearance rate, which is essentially the mass transfer coefficient  $K_g$  into  $C_B - C$  and that kind of equation; that has to be equated to number one, the reaction rate, if the reaction is only on the surface; or to the diffusive flux inside the catalyst palette, that is diffusion coefficient  $d$  times  $(\frac{dc}{dr})$  or whatever the flux term is; and then we have to write the balance for what is happening inside the catalyst palette; and for which we can use diffusion reaction equation and therefore, bring in our catalyst discussion into our reactor designed portfolio.

Following this, we looked at the energy balance in particular, to see what is, what happens when we have non isothermal reactor operations, so just as we have based on mass flow, we have batch reactors or continuous reactors, based on energy flow we can have two different extremes of reactions - one in which there is no energy removal from the system and adiabatic operation; or the other one where energy removal matches with

energy generation, there by maintaining the energy content of the reactor constant or ensure temperature is constant or is fixed; and that is a isothermal operation. So, isothermal operation and adiabatic operations are two extremes of non-isothermal reactor reactor design.

We followed this, up with few case studies, where we first of all looked at design of things like ethane cracking or hydrogenation of oil or ammonia synthesis, which lead us to the kind of reactors, reactor operations which are not does not follow in the category of isothermal or adiabatic. This primarily arises for those, reactions for which we have a reversible exothermic or even its irreversible exothermic exothermic reactions, where we saw that there is a conflict between the kinetics and thermodynamics; particularly, for exothermic reaction. The conflict takes this form, for attaining high equilibrium conversions, we need low temperatures; but to attain high reaction rates, we need high temperature. So, an isothermal operation with either high temperature or low temperature will not be good, because we will have to sacrifice on either one of them, either thermodynamics or reactor.

On the other hand, if we have adiabatic operation, the temperatures will keep rising from the initial starting point, if you are looking at a batch reactor or a fixed bed reactor; then what will happen is initial low temperatures, low kinetics, as temperature rise equilibrium is adversely effected, even though reaction rates may increase, but again therefore, we are we are in a situation, where both kinetics and thermodynamics has suffered. So, we saw how we can overcome this problem, by having there are several ways, one of them of was to have combination of adiabatic reactor followed, by heat exchanges.

So, you allow reaction to carry out in an adiabatic manner in a small bed, remove the energy that is generated, so heat exchanger follows it up with another small reactor, small bed and repeat it, so that, we get both high reaction rates and high equilibrium conversion. Now, we also saw that to achieve this, for exothermic reaction for example, you are to decrease the temperature from inlet to the outlet of the reactor, if you are using a fixed bed reactor or from starting time to end time, if you are doing a batch operation.

But this also leads to another type of operation, where the energy that is required, to increase the temperature at the beginning of the reaction, is the energy that is getting

generated, because reaction is proceeding; so, we combined heat exchange and reaction into a single step, in a cell and tube kind of arrangement, only changing the flow pattern that is, before reactants enter into reactor; they flow into the through the cell in such a manner, that the energy released from the reaction is taken up by the reactant molecules, before entering the reactor and therefore, they get preheated, just what we wanted. These operations we called them as auto thermal operations.

The third type of examples or class of examples, we saw was because of these non isothermal effects, our reactors are having sensitive behavior, what we term as parametric sensitivity? That is, a small perturbation can give rise to the reacting operation going from a safe to an unsafe operation; and this can take various different forms for example, in a batch reactor, you could have, that is the example of hydrogenous combustion, a safe operation to a reaction explosion. In a tubular reactor, you could have the example was highly in oxidation, you could have a case where what appear to be a normal operation, with temperatures all controlled.

Suddenly, somewhere in the reactor the temperature shoot up to a very high value; or runaway reaction, which could eventually lead to, if **if** the material is not able to withstand these temperature rises, it could be **it could be** catastrophic. Or in the stirred tank reactors, this led to what we called multiplicity of steady state, that is under same identical operating conditions; we could have more than one steady state in our **in our** reactor.

All these phenomenon, you did not have to bring changes in the operating conditions of a significant magnitude; few percentage point change in the cooling temperature or the initial partial pressure of the reactant; or the coolant temperature in a tubular reactor, is enough to go from a safe operation to an unsafe operation therefore, in design of reactors it is essential that, we identify these regions a priory, so as to completely avoid these unsafe **unsafe** operation.

Now, one may ask, why not go to the extreme and work in the regions when, there is **there is** complete even, if there is a 100 percent change in the operating condition, nothing will happen, we will still have a safe operation. That is ideal, but unfortunately, it turns out, that most of the reason where you get optimal performance of a reactor, be it

in the yields or selectivity or conversions, is dangerously close to these, this boundary between safe and unsafe operation.

Therefore, from practical point of view, we are forced to operate near that reason, but with a caution that, we should have good controls and detection systems. So, first of all detect the change in the operating condition and bring it under control as soon as it is detected. So, reactor design is invariably linked to good process **process** control; we then summarized or concluded our discussion, so we **we** looked at this parametric sensitivity behavior, multiplicity and therefore, looked at how we determine that, when there are more than one steady state possible, are they all stable.

Our definition of stability apart from the fact that there are formal definitions, but practical definition is if you have a steady state and you have a small perturbation and this important; that we can talk only for small perturbations, because all our analysis is was based on linearization of our non-linear dynamics.

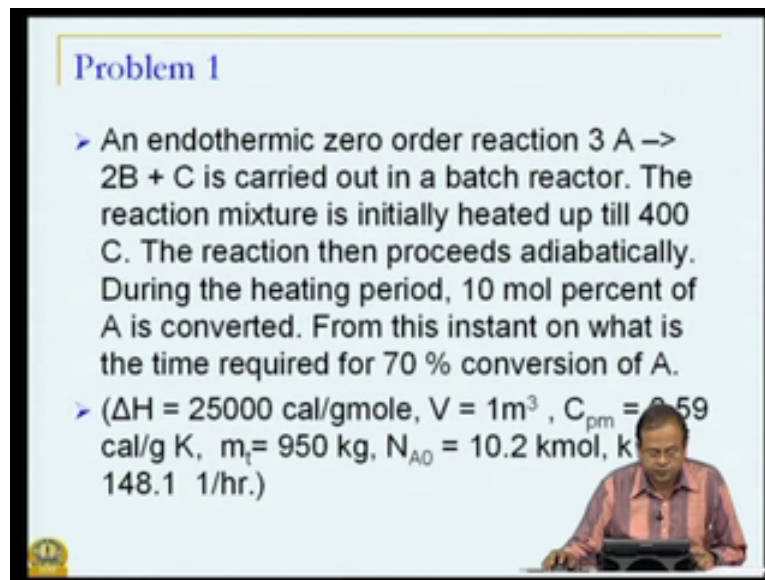
So, if you have perturbation and examine the performance of these perturbation; if that perturbation dies down that means, we return back to our original steady state from which, it was perturb then, we have what we call stable steady state.

If not we have a unstable steady state; that means, this perturbation keeps growing and there are formal ways namely looking at the Jacobian of the dynamic mass by an energy balances, looking at the Eigen values of this Jacobian matrix, at that particular steady state; and finding out whether the real part of the Eigen value is negative; then we have a asymptotical stable steady state.

And finally, we concluded our discussion on reactor design by looking at, how we can analyze the real reactors by using ideas of non ideal flow, age distributions, exit age distribution, internal age distribution, cumulative distribution, how we can determine it experimentally, and how it affects the performance of a reactor? We also saw that these age distributions or macro mixing alone does not determine the performance, because for the same distribution, you can get two different kinds of performances depending upon, whether the reactor a fluid element or the material inside the reactor, either interacts with each other or completely mixes or remains segregated or separated from each other.

So, not only the residence time distribution or macro mixing, but the earliness and the extent of these mixing or interaction is equally **equally** important or macro mixing is also equally important. So, with this summary, let us come to solving few problems on reactor **reactor** design.

(Refer Slide Time: 15:56)



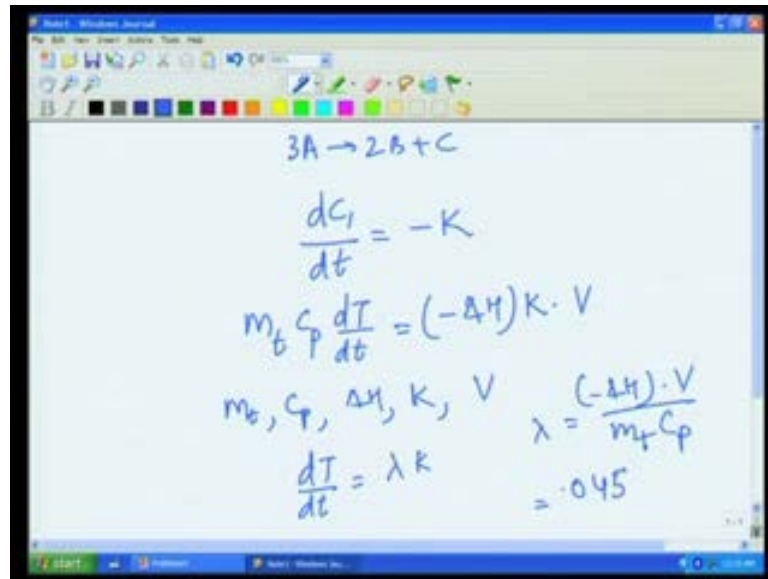
**Problem 1**

- An endothermic zero order reaction  $3A \rightarrow 2B + C$  is carried out in a batch reactor. The reaction mixture is initially heated up till 400 C. The reaction then proceeds adiabatically. During the heating period, 10 mol percent of A is converted. From this instant on what is the time required for 70 % conversion of A.
- ( $\Delta H = 25000$  cal/gmole,  $V = 1\text{m}^3$ ,  $C_{p,m} = 0.59$  cal/g K,  $m_t = 950$  kg,  $N_{A0} = 10.2$  kmol,  $k = 148.1$  1/hr.)

The first problem, that we will look at, is a example of endothermic 0 order reaction  $3A$  going to  $2B$  plus  $C$ , is carried out in a batch reactor. The reaction mixture is initially heated up to 400 degree centigrade, reaction then proceeds adiabatically; during this heating period 10 mol percentage of  $A$  is converted. And from this instant onwards, what is the time, that is required to obtain 74 percent conversion of  $A$ ; and then there is some data that is **that is** given.

So, let us try to look at, what is the important information that is given, kinetics is 0 order, reaction is given, batch reactor initial temperature adiabatic reaction initially, during this heating period 10 mol percent is **is** converted from this instant; that means, what is the time that is required for 74 percent conversion of  $A$ . So, we need to find time, we have been given heat of reaction adiabatic, endothermic reaction, the volume of the reactor, the specific heat of the reacting mixture, which is given constant the total mass initial moles and the rate constant, which turns out to be the rate of reaction; because it is a 0 order reaction. So, let us try to work this problem off and look at **look at** how we go about solving this.

(Refer Slide Time: 17:56)



Our reaction is 3 A going to 2 B plus C, no change in number of moles, so whether it is a gas phase reaction or liquid phase reaction; we the volume can be assume to be constant and so, with that assumption we can write the mass balance as  $dC_1/dt$  equal to simply minus K, that is the rate of rate of reaction. What about the energy balance? We can also write, since, we have been given the total mass and the specific heat, so energy content can be  $m C_p dT$  by small  $d t$ , that is energy accumulation term which will be nothing but, minus delta H into the rate of reaction into the volume of the reacting **reacting** mixture, **right**.

We have been given  $m_t C_p \Delta H K V$  everything is given to us. So, for the, **for the** first **first** part we can write  $d T$  by  $d t$  as  $\lambda$  into K, where  $\lambda$  is minus delta H into V divided by  $m_t$  into  $C_p$ . So, if you put all those numbers together that works out to be 0.45. All the information is **information is** given to us, mass balance, energy balance, they are related.

(Refer Slide Time: 19:51)

Handwritten notes on a whiteboard:

$$T = T_0 - \lambda(C - C_0)$$

$\lambda, T_0, C_0, C$

$$T_{10min} = 78.7 \text{ C}$$
$$\frac{dT}{dt} = \lambda k$$

$t = ?$

$$\frac{dT}{dt} = \lambda k$$
$$K(T) = A e^{-\frac{E}{RT}}$$

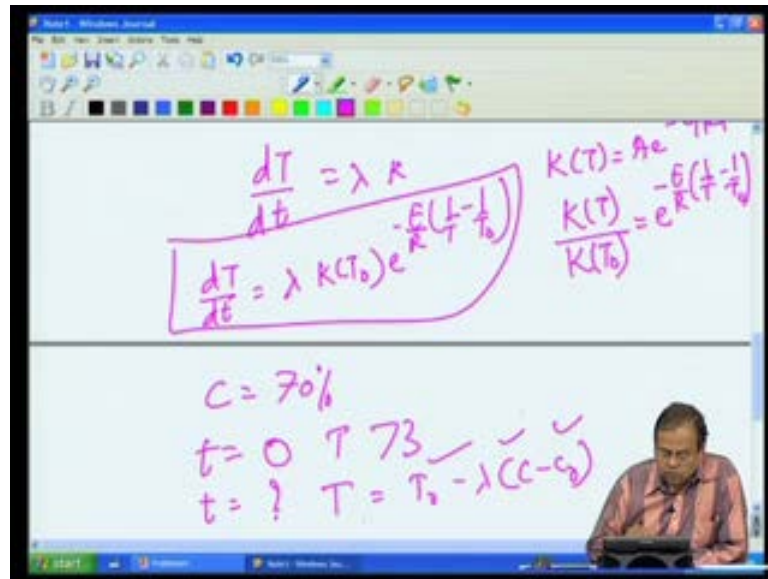
So, we can put them together and say  $dT$  by  $dt$  plus  $\lambda dC$  is equal to 0. So, with initial concentration at time  $t$  equal to 0, if you say that it  $C_0$  and temperature is  $T_0$ ; then we can integrate these equation and write  $T$  is equal to  $T_0$  minus  $\lambda$  into  $C$  minus  $C_0$ , now what was the first piece of information that was given to us? It was given to us, that during the initial heating period conversion is given that means, we know the initial concentration conversion is know, so we know  $C_0$ , we know  $C$  and this time the temperature will obviously, go down, because it is an endothermic reaction. So, knowing this energy balance, so what has been given we know  $\lambda$ , we know what is  $T$ , we know what is  $C_0$ , and we have also been given this. So, from these four pieces of information, we can calculate what will be the  $T$  at the end of 10 minutes, because all these information is known and that value works out to be 78.7 C that is **that is that is** the information that is **that is** available.

Now, what happens afterwards, because what is the problem then? The problem is we want to find out, what is the time required for 70 percent conversion, remember we have been given only the rate constant at 1 temperature; that is **that is** 400, we do not know what that, what is the activation energy and so on. So, now, if we go back and look at our energy balance, is **is**  $\lambda$  into  $k$ , so I what **I what I what I** want to find out, what is what is the time required for 70 percent **70 percent** conversion. When the conversion is 70 percent, I can calculate what will be the temperature; so, I want to find what is the time, so this one, we can now write  $dT$  by  $dt$ ,  $\lambda$  value we know and let us assume



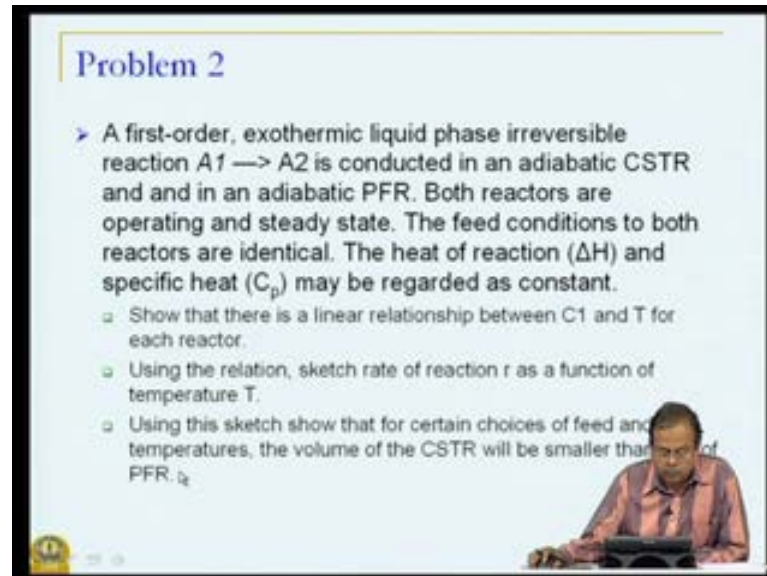
erroneous erroneous rate form, erroneous rate form for K, so let us assume K of T is a e raise to minus e by r T or we can write K of T with K of T at some reference temperature that is known to us as, e raise to minus e by r into 1 by T minus 1 by reference temperature, that is that is known to us; or in other words using this information the reference temperature that is known to us is 400.

(Refer Slide Time: 23:42)



So, I can write 1 by 1 by T naught the activation energy is also given or not, it should have been given, so let us assume the activation energy is also given otherwise, we cannot solve this problem. So, knowing this we can we can actually integrate these equation, this is exponential in in temperature; if activation energy was given to us has to be given to us. So, the problem is when conversion is 70 percent, we can calculate what should be the temperature, because we know this linear relationship. So, knowing this at time T equal to T equal to 0, our temperature was something like 6 or 73 point something. So, what will be the temperature time when that new temperature which was T naught minus lambda into C minus C naught we know all all these quantities. So, we can calculate that and find out the find out the temperature.

(Refer Slide Time: 25:20)



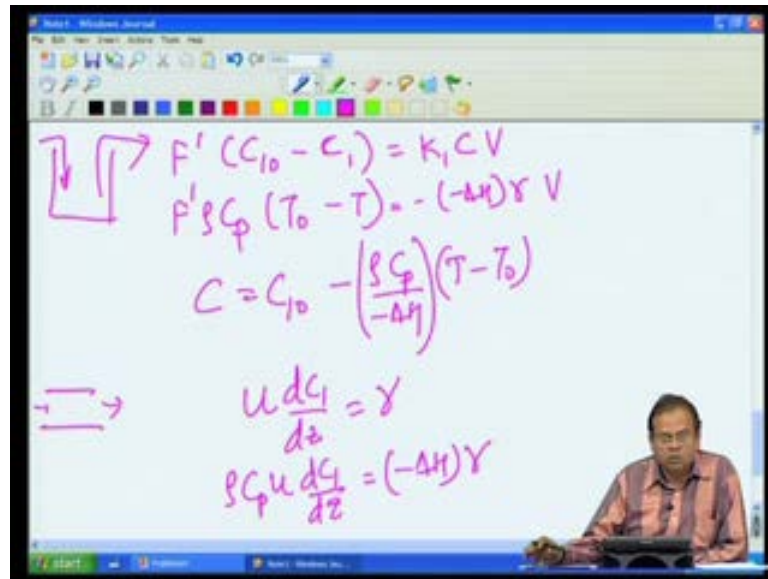
**Problem 2**

- > A first-order, exothermic liquid phase irreversible reaction  $A_1 \rightarrow A_2$  is conducted in an adiabatic CSTR and in an adiabatic PFR. Both reactors are operating and steady state. The feed conditions to both reactors are identical. The heat of reaction ( $\Delta H$ ) and specific heat ( $C_p$ ) may be regarded as constant.
  - Show that there is a linear relationship between  $C_1$  and  $T$  for each reactor.
  - Using the relation, sketch rate of reaction  $r$  as a function of temperature  $T$ .
  - Using this sketch show that for certain choices of feed and exit temperatures, the volume of the CSTR will be smaller than that of PFR.

It is a fairly simple straight forward **straight forward problem**; let us look at another problem. This problem and this problem again let us look at this problem a first order exothermic liquid phase irreversible reaction  $A_1$  to  $A_2$  is conducted in an adiabatic CSTR and in adiabatic plug flow reactor; so, we have two different reactors and we want to probably compare their performances.

Both reactors are operating at steady state, so we have been given adiabatic CSTR and adiabatic plug flow reactor, so probably we want to compare the performance of this two, both are at steady state feed conditions are exactly identical, heat of reaction and specific heat can be taken as constant; we have to show that for both these reactors, there is a constant relationship between concentration and temperature, using this relationship find out or sketch the rate of reaction as a function of temperature; and using the sketch, so that for certain choices of feed and exit temperatures; the volume of CSTR will be smaller than that for plug flow reactor. So, let us see how we go about solving this problem, all right.

(Refer Slide Time: 27:06)



So, we have a stirred tank reactor first, so let us write down the mass balance,  $F'$  into inlet minus outlet concentration, must be same as  $K_1$ , first order reaction and the energy balance  $F' \rho C_p (T_0 - T) = -(-\Delta H) \gamma V$ , why because adiabatic reactor, so there is no heat added or removal **removal removal** term. So, now we can **we can** combine this two, assuming all properties are **properties are** constant and we will get  $C = C_{10} - \frac{\rho C_p}{(-\Delta H)} (T - T_0)$  minus  $T$  naught.

What about tubular reactor? A tubular reactor mass balance  $u \frac{dC_1}{dz} = r$  rate of reaction and  $\rho c_p u \frac{dC_1}{dz} = \text{minus } \Delta H \text{ into } r$ , again no heat added or removal term.

(Refer Slide Time: 28:43)

Handwritten mathematical derivation on a whiteboard:

$$C = C_0 \exp\left(\frac{-\Delta H}{\rho C_p \alpha z}\right)$$

$$\Rightarrow u \frac{dC}{dz} = -\gamma$$

$$\rho C_p u \frac{dC}{dz} = (-\Delta H) \gamma$$

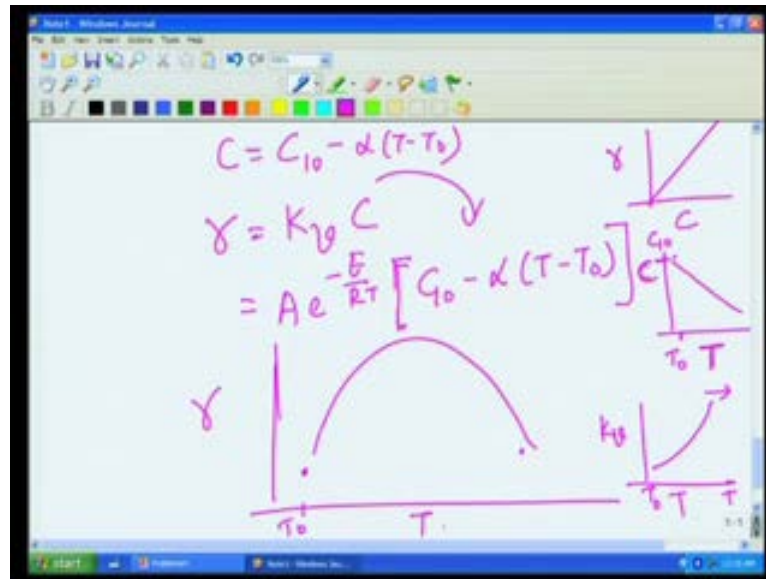
$$(-\Delta H) \frac{dC}{dz} + \rho C_p \frac{dT}{dz} = 0$$

$$C = C_0 - \left(\frac{\rho C_p}{-\Delta H}\right) (T - T_0) \leftarrow$$

$\alpha$

So, we can **we can** combine this two equations minus  $\Delta H \frac{dC}{dz}$  plus  $\rho C_p \frac{dT}{dz}$  equal to 0; and again if you take the same **same** approach, we will get  $C$  equal to  $C_0$  minus  $\rho C_p$  by minus  $\Delta H$ ,  $T$  minus  $T_0$ . So, if we now compare the relationship for stirred tank reactor and for plug flow reactor, we have shown that there is a linear relationship, only if properties or there such as  $\Delta H$ ,  $C_p$ ,  $\rho$  are constant let us make that **let us make that** assumption. And let us call this constant  $\alpha$ , so what we have is  $C$  is  $C_0$  minus  $\alpha$  into  $T$  minus  $T_0$ . So, what is this next problem? So, we have **we have** got the linear relationship between  $C_1$  and  $C_1$  and  $T$  using this relationship sketch the rate of reaction as a function of temperature. So, what we have is a first order reaction.

(Refer Slide Time: 30:16)



So, rate of reaction is  $K V$  into  $C$  where  $K V$  is function of a temperature and from this relationship we also know  $K$  can be expressed as temperature. So, we can write this **this**  $K V$  as erroneous form into  $C 10$  minus  $\alpha$  into  $T$  minus  $T_0$ ; remember this has come from **come from** this  $T$ , now what kind of **kind of** reaction is given, exothermic reaction if it say exothermic reaction what is the sign of  $\alpha$ , from here it is a positive **positive** **positive** number, what it **what it** means, what does it mean in a reaction reactant concentration is always going to decrease and exothermic adiabatic reactor temperature is always going to increase; that is **that is** what we should keep in mind.

So, what we have to sketch is rate versus temperature, now we do not have any numbers, so difficult to **difficult to** actually plot it, but let us qualitatively try to see how it will **it** **will** look like, now we know how rate will look as a function of concentration; if temperature was constant a linear curve, so it will always always increasing. So, what it implies is rate is govern by this two factors  $K V$  and  $C$ . Now, how does we know this we also know that rate as a function of temperature is an exponentially increasing function, because as temperature increases the rate constant increases we know all that, but our problem is to find rate as a function of temperature.

So, first let us try to see, how rate or concentration will change as **concentration will** **change as** temperature. So, here we take help of these equation if my temperature is  $T$

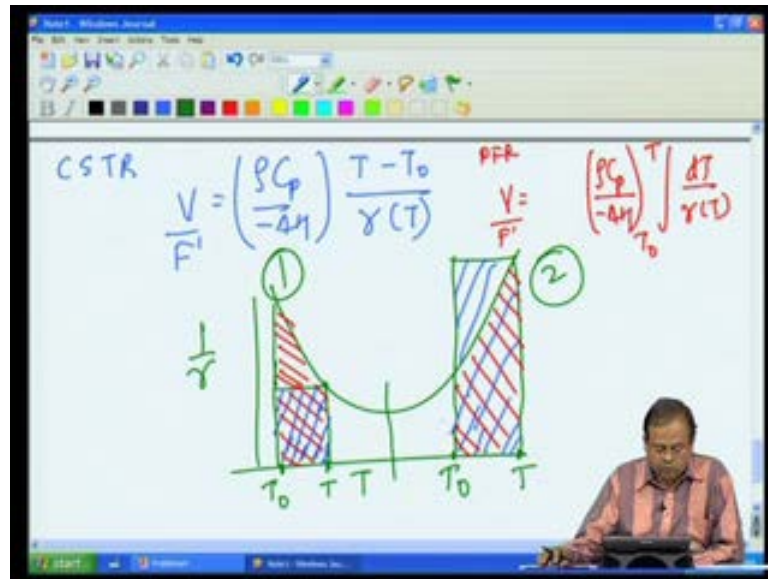
naught or the starting temperature let us say what will be my concentration concentration will be  $C_1$  naught this value.

Now, what happens as my temperature increases, since, it is exothermic reaction, the concentration decreases in a linear manner. So, this is how concentration changes with temperature, let us try to see how  $K_V$  changes with temperature and we know this; there will be some increasing function like this, starting with  $T_{naught}$  to a higher **higher** value. So, what we are interested in knowing is how the product of these two values  $K_V$  into  $C$  looks like, because that is nothing but the **nothing but the** rate.

So, qualitatively, we can see when  $T$  is near  $T_{naught}$ ,  $K_V$  is a low value even though  $C_1$  naught is a low value, the product is likely to be a low value. When  $T$  is very large,  $K_V$  is very large, but  $C$  is very small. So, again product is likely to be again a low value  $K_V$  as a function of time, a temperature is a continuous function,  $C$  as a function of temperature, it is a continuous function. So, a continuous function which has low values at both extremes of temperature must go through a peak and therefore, our rate versus temperature we look something like this, so that is my sketch.

Now, using this sketch, so that for certain reactions the feed or choices of feed and exit **exit** concentration, the stirred tank reactor will be better than plug flow reactor, now how do we show that; remember this is my rate versus temperature now let us go back to our **let us go back to our**, mass balance equation, first stirred tank reactor along with the fact that  $C$ , which appears in this  $r$ , which is  $K_V$  into  $C$  is a linear function of temperature. So, what will be my energy balance, my mass balance actually instead of mass, I can work with my energy balance, let us to illustrate the same idea.

(Refer Slide Time: 35:47)



So, for CSTR **for CSTR**, I can write that equation and you can verify it for yourself,  $\rho C_p$  by minus  $\Delta H$ , which is actually our  $\alpha$  value into  $T - T_0$ , divided by  $r$  of  $T$ ; and for plug flow reactor **for plug flow reactor**, this volume will work out to be  $A$  into  $u$ , cross sectional area into velocity divided by  $\rho C_p$  into minus  $\Delta H$  into integral by  $r$  of  $T$  from  $T_0$  to  $T$ . So, our usual method of comparing the two reactors - plug flow and CSTR can conveniently be used for this case **this case** as well, what is that usual **usual** way? We see that; it is determined by one over one  $r$ , so from this  $r$  versus that is rate versus temperature, let us construct one over  $r$  versus temperature.

It will be an inverted figure of this  $r$  versus temperature, so we have this, with  $T_0$  being being this world. Now, what is the volume required in a stirred tank reactor? In a stirred tank reactor that **that** volume is for example, if this is my  $T_0$  and this is my  $T$ , desired  $T$ , then what will be that **what will be that** volume;  $T - T_0$   **$T - T_0$**  divided by **divided by**  $r$  of  $T$ , so  $T - T_0$ ; that means, area of these rectangle, so this is my C S T R volume.

What is my plug flow reactor volume? It is the area under the curve one over  $r$  versus  $T$ , between the limits  $T_0$  to  $T$ ; and what is that area under the curve? That area under the curve is this area. So, what will be the volume for plug flow reactor? This whole volume, the red color volume, so now, you can see for this plug flow reactor volume, which is area under the curve is much larger than the reactor volume for stirred tank

reactor. So, that is **that is** the case when stirred tank reactor is **reactor is** better than **better than** plug flow reactor, but what if my  $T$  naught was here, how do I determine those limits as what we are trying to look at.

Suppose my, so this is my one scenario, let us look at another scenario, if my  $T$  naught is here and my  $t$  obviously, temperature is higher than the inlet, because exothermic reaction; so, what will happen to my reactor volumes, now let us look at the stirred tank reactor first the stirred tank reactor, now the volume required will be one over  $r$  of  $T$  that is this much multiplied by  $T$  naught into  $t$  that means, my reactor volume will be these entire **entire** area; and proportional because there is a constant  $\rho c_p$  by minus  $\Delta h$ . So, that constant is **is is is** understood.

Now, what about **what about** the plug flow reactor? For a plug flow reactor area under the curve is now only this much area. I should **I should**, I think stand corrected, this should be  $F$  prime and let us put it in the same manner, so that there is no confusion we are essentially looking at the naught, the looking at the residence type. So, what happened now in this scenario two, what do I see? I see that, if area under the curve now is smaller than the area of this rectangle; that means, plug flow reactor is better than stirred tank reactor. So, depending upon our initial choice of starting temperature, if it was up to here right and in fact, all those cases were initial temperature was **was** here or even little more beyond, we will find that stirred tank reactor is better, but for other cases such as second case, thus plug flow reactor will be better than stirred tank **stirred tank** reactor.

The third problem is actually very similar, to what we just now saw, so what was the reason, why this behavior occurred that stirred tank reactor better than plug flow reactor; the reason was that we had a rate and temperature dependency which was of this non-monotonic form, but this non-monotonic form can come from rate as a function of concentration also and that is what this problem is, that is a perfectly mixed stirred tank reactor is to be used for reaction and is operate isothermally, so no temperature variations.



(Refer Slide Time: 42:16)


**Problem 3**

> A perfectly mixed stirred tank reactor is to be used for the reaction and is operated isothermally. The reactor is  $20 \text{ m}^3$  in size and the feed rate is  $0.4 \text{ m}^3/\text{s}$  with a concentration of  $C_{10} = 13 \text{ kmol/m}^3$ . The rate expression for the reactor is

$$r = \frac{C_1}{(1 + C_1)^2}, \text{ kmol / m}^3 \cdot \text{s}$$

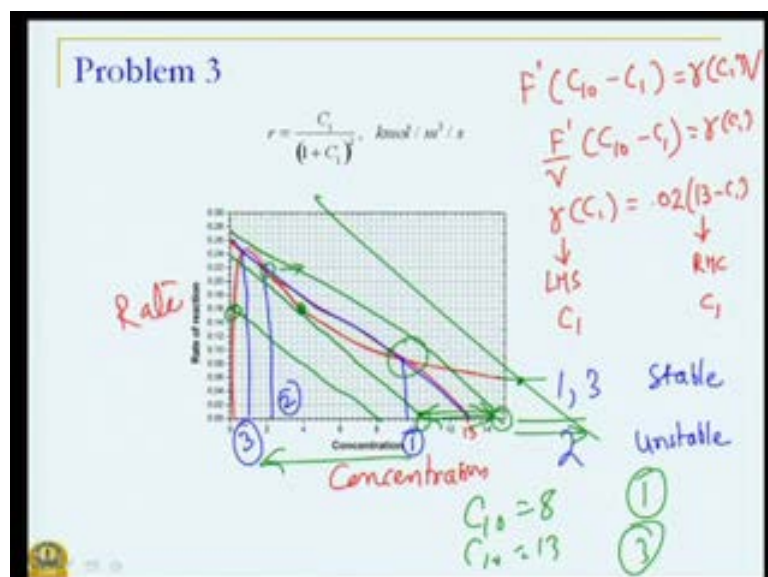
> It is suspected that the operation may have regions of unstable operation with multiple steady states.

- Determine whether this is indeed the case
- Outline a procedure to determine how the feed concentration should be changed to avoid the problem.



The reactor volume is given **reactor volume is given**, so which highlight the information that is given, the flow rate is given, inlet concentration is given and the rate expression is given; the question is it is suspected that the operation may have regions of unstable region with multiple steady states, determine whether this is indeed the case outline the procedure to determine, how the feed concentration should be changed.

(Refer Slide Time: 43:14)



So, that this problem does not **does not** arise now let us try to **try to** look at this. So, what is this rate expression? This rate expression is what is actually shown here, in this

particular figure; and it is again a non-monotonic function. So, it is an isothermal, so rate versus concentration is now a non-ideal **non ideal** behavior. So, what is our question we want to find out whether there are multiple steady states possible and how to do we determine feed conditions, so that multiple steady states do not occur that is our **that is our** problem.

So, let us try to **try to** take a look at solution of this **of this** problem, isothermal, so we just need to look at mass balance and if we take again our mass balance  $F' = C_1(0 - C_1) - r$ . We have been given  $F'$ , we have been given  $C_1$  and **and** the all those **all those** quantities. So, we can actually write  $F'$  by  $V$  into  $C_1(0 - C_1) - r$  and if you put all those values  $r$  of  $C_1$  is 0.02 into  $13 - C_1$ ; that is just some **some** number. We can of course, put that  $r$  rate expression and try to solve for  $C_1$  and so on, but let us **let us** look at this solution in a graphical way.

So, now, graphical means what we have left hand side as a function of  $C_1$ , we have right hand side as a function of  $C_1$ , so let us plot that and the left hand side is already plotted the rate versus  $C_1$ , how will the right hand side **how will the right hand side** look like for this particular case right hand side is nothing but, the straight line starting with  $C_1$  of 13 suppose this is that 13, right hand side is 0. So, this is a 13 point, what happens when  $C_1$  is 0 into 13 into 0.02, that is 0.26.

So, this is another point and a straight line I will do my best to draw a straight line between these two points. So, what has happened, what will be the steady state solution when left hand side equals right hand side? So, let me draw it again with another color. So, what is the possible **possible** steady state, steady state number 1 steady state number 2 and a steady state number **number** 3. So, these are the possible **possible** steady state **to** this solution; so, again multiple **multiple** steady state.

Now, in this particular case, I would not go into the match, but you can work it out yourself about the stability for example, remember when we talked about isothermal, non-isothermal reactor, we said that for those conditions under which rate of energy removal is higher than the rate of heat generation; we had a problem, that is or other we had a stable steady state; and when the heat of generation was slope was higher than the removal, we had an unstable steady state, here there is no energy removable of generation,

but what is it is mass generation and mass removal, if you look at left hand side, it is nothing but mass generation or rate of mass conversion or the rate of reaction and the right hand side is nothing but mass in and out, net mass added to the system or removed from the system, which ever we want to look.

And the steady state is a balance between the two which is what we what we expect. So, based on the discussions that that we had we can safely say and you can verify it, that 1 and 3 are stable and 2 is unstable. Once again how do we **how do we** verify it. So, let us say that we have this steady state number 2 and we introduce a perturbation, **we introduce a perturbation** what will happen? In this particular case the rate of conversion of one species is lower than the rate of its net addition.

So, what will happen? Concentration will keep on increasing and we will come to this particular steady state and same thing can be argued, if the perturbation is in the reverse direction, so now, how do we determine, how to avoid this; that means, the intersection of this two points at these two curves, right hand side and left hand side must be a single point; what does it **what does it** depend on? It depends upon the slope 0.02, but what is our question, we want to find out under what conditions feed concentrations it should remain on changed.

So, we keep feed rates same, but we change this **change this change this** feed concentration from 13 to a different value. So, suppose I make it 8, the slope is same as this blue line and 8, so 0.16, so we will have this as an operating line and the intersection point is only 1. So, between 8 and 13, 8 we had only that is feed concentration, that is  $C_1$  naught equal to 8 only one steady state if or  $C_1$  naught is thirteen we had 3 steady states.

So, between these two, there must be a point, where we shift from one steady state to 3 steady state and what would that point be? That point would be where, this operating line with a slope is just tangent, that is that straight line is tangent to our reaction rate curve, that will be one limit, but that tangent can be found at two different locations, so another tangent over here, so in this feed concentrations, we can work out what those exact numbers are in this region we will have 3 steady state, any feed concentration on this side, if you do you will have only one steady state intersection.

So, any anything here or here single steady state, but all those concentrations in between us have 3 steady states, so again you can you can calculate the multiplicity by actually calculating the Eigen values and so on. In this case, it is only one dimensional, so Eigen value calculation is even more easy, so with this we will come to the conclusion of our course by. So, we the last lecture was essentially looking at some problems I thoroughly enjoyed giving this giving this lectures, I hope you find them useful too thank you.