Chemical Reaction Engineering

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Module No. #05

Lecture No. #29

Non Isothermal Reactor Operation

Let us continue our discussion on adiabatic reactors and just to recap, let us write down the energy balances for two types of reactors and we will take forward from there. So, we have, let us say, the stirred tank reactor.

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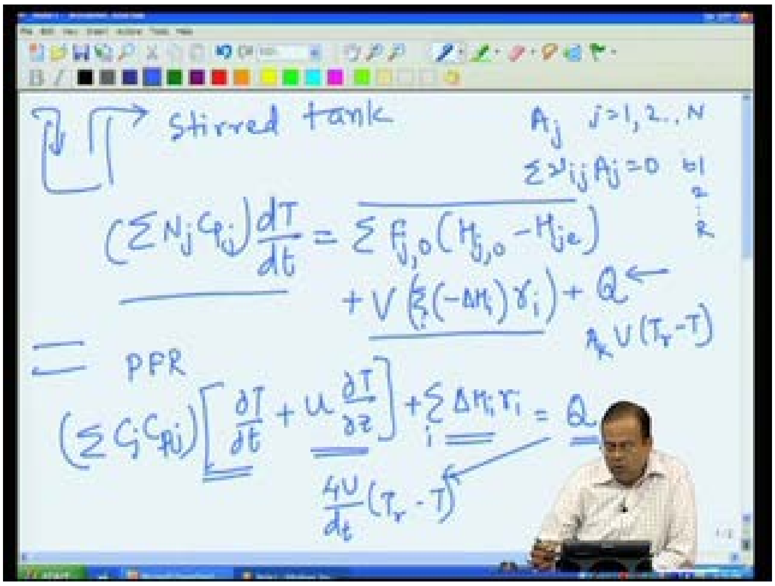

Stirred tank

$A_j \quad j=1,2,..,N$

$\sum \nu_{ij} A_j = 0 \quad i=1,2,\ldots,R$

$$\left(\sum N_j C_{pj}\right)\frac{dT}{dt} = \sum F_{j,0}\left(H_{j,0} - H_{je}\right) + V\left(\sum_i (-\Delta H_i) r_i\right) + Q$$

$a_v U(T_r - T)$

PFR

$$\left(\sum C_i C_{pi}\right)\left[\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial z}\right] + \sum_i \Delta H_i r_i = Q$$

$\frac{4U}{d_t}(T_r - T)$

So, for a stirred tank reactor, stirred tank we have the energy balance which looks something like this. Remember our reaction is, there are large number of reactions let us say, in number of species A j, j going from 1, 2 up to N and we have a reaction summation u i j A j equal to 0, where this is my I th reaction. So, I can go from 1, 2 up to let us say, independent reaction R. So, we have all the species, we have these reactions taking place between the species and if we consider ideal reactors, stirred tank reactor, the energy balance boils down to this summation N j C p j. So, this is my energy accumulation term. N j is the most of species j, C p j is the specific heat; we had derived this equation in earlier classes, so, this is equal to summation F j 0; F j 0 is the molar flow rate of species coming inside.

So, we are considering a general stirred tank reactor with a continuous operation and A j is the enthalpy, subscript o denoting the entry point and e denoting the exit point. So, the accumulation is a result of the energy difference between the stream coming in and going out plus there are reactions taking place and each reaction has a heat of reaction delta I, the ray reaction is taking place at a rate r i and some over all these reactions I will be the total energy that is generated in the in the system. So, that is a contribution of reaction plus whatever energy we are adding to the system. So, q for example, we can also write as A k U into T r minus T where A k is the area of a retransfer, U is the overall coefficient of heat transfer, T r is the temperature of the coolant or the heating media that is in the jacket or which is transferring heat adding heat and T is the temperature, so, this is this is the energy balance for stirred tank reactor.

We can also write energy balance for a plug flow reactor in a very similar similar manner as summation C j C p j into I am writing an unsteady state balance plus is equal to Q, where Q in this tubular reactor for example, if you have a tubular reactor, we can write as where U is again the heat transfer coefficient, d t is the diameter of the tube, T r again is the temperature of the media which is cooling or heating the reactants and T is the temperature inside. So, essentially in both these cases, the idea is accumulation for example, is a result of convective heat transfer, the heat generated in the reaction and heat which is externally added to the system; a similar term in the plug flow reactor, the accumulation term, the convective energy transport, the generation term and the heat addition term. So, these are our general energy balances and now, let us look at a simple, reaction simple reaction that is single reaction in an adiabatic reactor. Now, if you have an adiabatic reactor, what will happen if we are not adding or removing any heat? So, q terms will be 0 and the remaining appropriate terms will will will remain.

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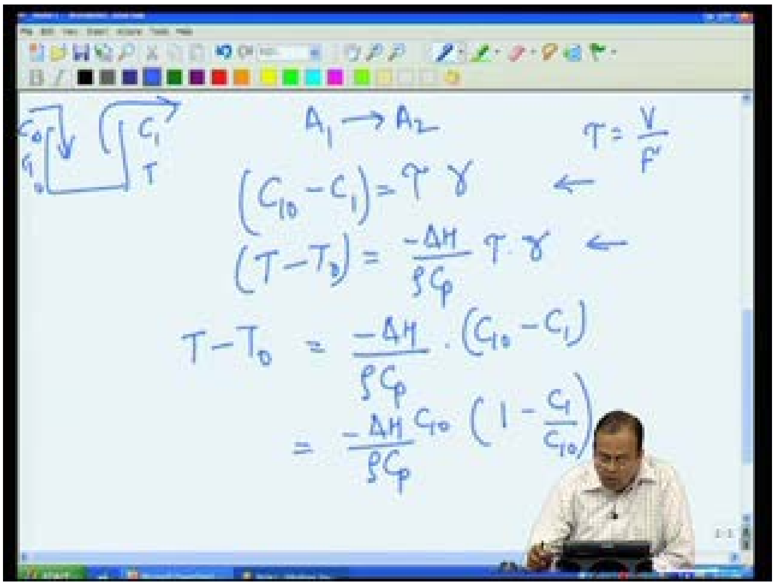

$$A_1 \rightarrow A_2 \qquad \tau = \frac{V}{F}$$

$$(C_{10} - C_1) = \tau \, r \leftarrow$$

$$(T - T_0) = \frac{-\Delta H}{\rho C_p} \tau \cdot r \leftarrow$$

$$T - T_0 = \frac{-\Delta H}{\rho C_p} \cdot (C_{10} - C_1)$$

$$= \frac{-\Delta H}{\rho C_p} C_{10} \left(1 - \frac{C_1}{C_{10}}\right)$$

So, let us consider a reaction A 1 going to A 2 A 1 going to a 2 and let us say that it is occurring in a stirred tank reactor stirred tank reactor, C naught and T naught are my inlet concentration and temperature C 1 and T is my exit concentration and temperature and we will consider a steady state balance. So, accumulation is is is is not there is equal to zero. So, we are considering steady state balance. So, we will put this term to 0 and adiabatic operation this term to 0 and then we will consider both mass and energy balances and we can write C 1 0 minus C 1 minus C 1 as equal to tau into r, what is T a u tau is our volume divided by the volumetric flow rate or the residence time. So, this is our mass balance and now, if we assume that the property that is in this energy balance in this energy balance we will write A j enthalpy as C p into T temperature terms and we will assume those property are constant and define the mixture property. Then we can write energy balance, simplify that energy balance as minus delta H by rho C p into tau into r.

So, essentially what we have done is, we have considered a single reaction, we have written the enthalpy of the of the mixture in terms of its density and specific heat of the mixture rather than considering individual component and if then you rearrange we will get this kind of kind of term. Now, this is our energy balance, this is our mass balance and if we assume all properties such as C p rho r are constant, we get we get this this this particular balance and let us try to simplify this further. So, what we will now do is combine this mass and energy balance because we see this tau r term which is common.

So, we can write delta H by rho C p into C 1 0 minus C 1 that is, instead of instead of instead of tau r, we will write it as C 1 0 minus C 1, which I can further simplify as minus delta H into C 1 0 by rho C p into 1 minus C 1 by C 1 0 or C 1 0 minus C 1 by C 1 0 which according to our definition of conversion is nothing, but the conversion.

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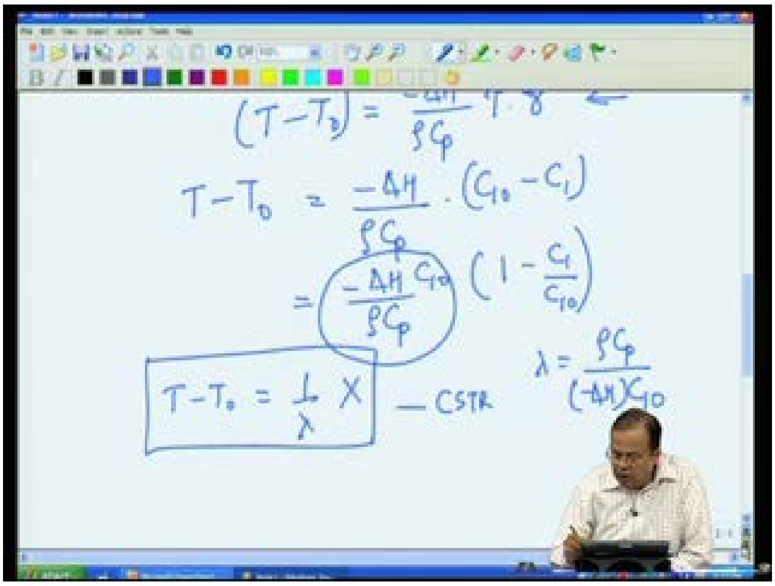

$$(T-T_0) = \frac{-\Delta H}{\rho C_p} \tau \cdot r \leftarrow$$

$$T-T_0 = \frac{-\Delta H}{\rho C_p} \cdot (C_{10}-C_1)$$

$$= \frac{-\Delta H \, C_{10}}{\rho C_p} \left(1-\frac{C_1}{C_{10}}\right)$$

$$\boxed{T-T_0 = \frac{1}{\lambda} X} \text{ — CSTR}$$

$$\lambda = \frac{\rho C_p}{(-\Delta H) C_{10}}$$

So, I am going to now write this energy balance as T minus T 0 as I am going to define this quantity as 1 over lambda and write this as into X, x that is our conversion. What is what is lambda? our lambda as we have defined is rho cp divided by minus delta H into C 1 0. So, this is our relationship between temperature and conversion for an adiabatic reactor for a single reaction taking place in an adiabatic reactor. What does this relationship tell us? It tells us that temperature and conversion are linearly related through this constant 1 over 1 over lambda. There are certain assumptions that we have made, namely the properties of such as C p rho delta H are not temperature dependent, they are constant they are defining this properties for a mixture, but under this under this simplifying conditions if they are satisfied and a reasonable assumption to do is at least to illustrate certain important features of adiabatic adiabatic operations. So, we get this for stirred tank reactor ok.

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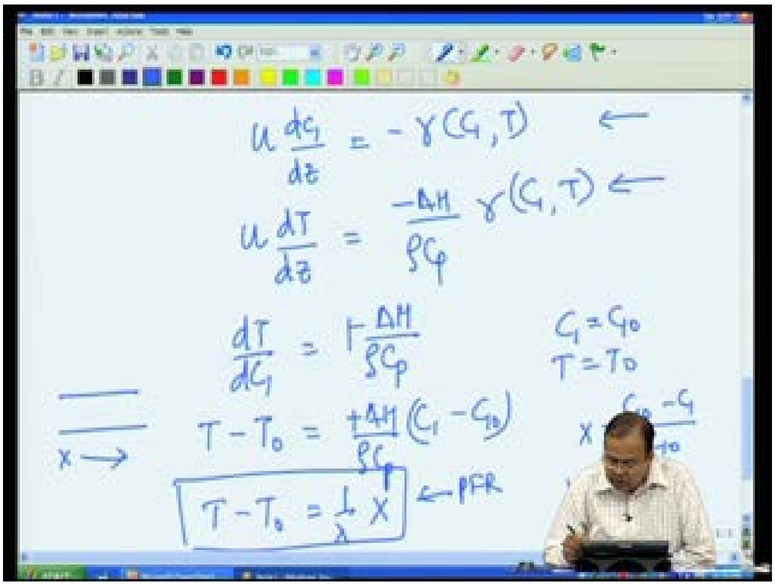

Let us try to do the same thing for a plug flow reactor or a tubular tubular reactor. Now for tubular reactor, same reaction we have mass balance equation which looks u d C 1 and d t again I am doing a steady state balance, no dispersion or dispersive flow because we looking at ideal reactor operation and similarly, we can therefore, write the energy balance just as we wrote mass balance as minus delta H rho C p r of C 1 and T. That is, what essentially we are doing is, we are now simplifying this plug flow energy balance for adiabatic operations. So, q is 0 steady state operation. So, delta T dau T of T temperature is is 0 and we are just rearranging these terms only instead of writing it as individual properties of the mixture, we are defining properties of the mixture namely C p rho and so on, so we get this kind of kind of mass balance.

So, we have our mass balance, we have our energy balance and now, we can once again combine this and say d T by d C 1 from this particular relationship is nothing but delta H by rho C p, which I can integrate saying that at the inlet, C 1 is C 1 0, T is T 0. So, I can integrate this and write T minus T 0 as minus delta H rho C p into C minus C 1 minus C 1 0 and once again, I can I can write the same relationship the same relationship, as I think this should be plus. So, here. So, I can I can once again write T minus T 0 as 1 over lambda into X by recognizing that X is C 1 0 minus C 1 by C 1 0 and lambda is rho C p by minus delta H into in to C 1 zero, so this is my relationship for plug flow reactor. So, what is happening in the plug flow reactor? Also, once again temperature and conversion are linearly related to each other, essentially temperature and concentration, but we can write it as temperature and conversion, this is for plug flow reactor.

Few minutes back, we defined the same relationship for a stirred tank reactor and we saw that for a stirred tank reactor also the same relationship applies. But one thing that we have to remember even though the relationship is same is that is temperature and conversion are linearly related. There are two different ways in which this is happening; In a stirred tank reactor, the temperature inside the reactor as well as in the exit is constant and so is the concentration and therefore, this is a single value relationship whereas, for tubular reactor or plug flow reactor, conversion is changing along the length of the reactor. So, X is changing along the length of the reactor and so is the temperature. But the way temperature and conversion are related, remains same. That is, the relationship is same but these have two different meanings or interpretations of what is happening in the in the reactor.

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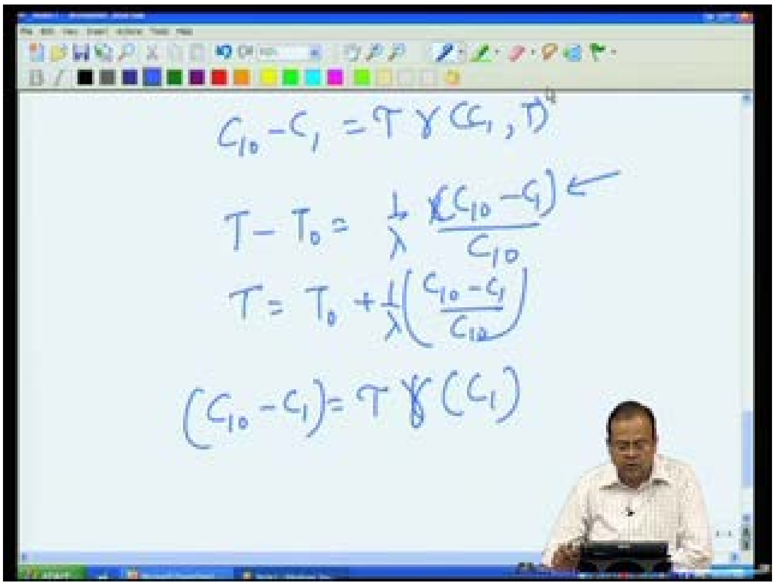

$$C_{10} - C_1 = \tau\, r(C_1, T)$$

$$T - T_0 = \frac{1}{\lambda}\,\frac{(C_{10} - C_1)}{C_{10}} \leftarrow$$

$$T = T_0 + \frac{1}{\lambda}\left(\frac{C_{10} - C_1}{C_{10}}\right)$$

$$(C_{10} - C_1) = \tau\, r(C_1)$$

So, now, what what this how how does this help us? Remember, if you all look at for example, C H T R, we have our balance which is C 1 and T. But we also know T is related to the concentration or conversion or I can write this as C 1 0 minus C 1 by C 1 0 or in other words, I can write temperature both in case of stirred tank reactor and plug flow reactor in terms of concentration alone. And thereby, now my mass balance equation is simply r of C 1 because I can eliminate temperature in terms of C 1. It is not a simple simple relationship but nonetheless, we have a single relationship that suffices to account for both mass and what energy energy balances. Why is that possible? It is possible because we have mass balance and we have combined mass and energy balance and therefore, we can eliminate concentration in terms of terms of temperature or temperature in terms of concentration.

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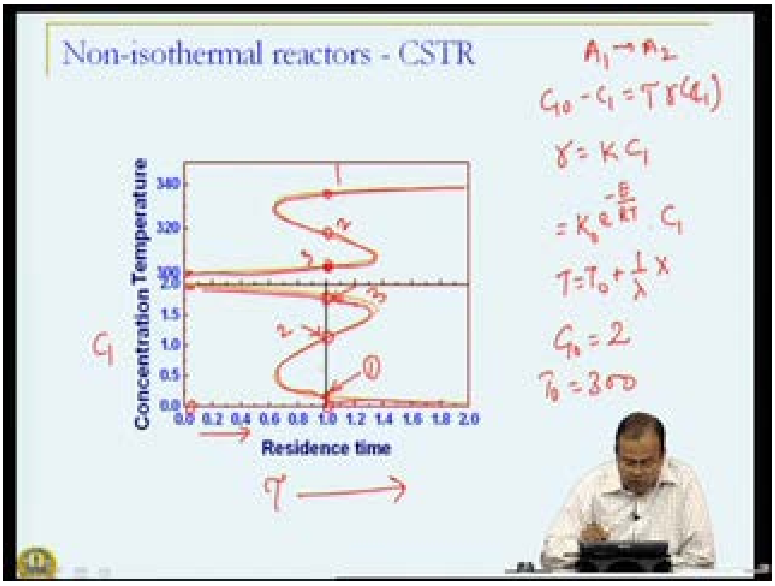

Non-isothermal reactors - CSTR

$A_1 \to A_2$

$C_{10} - C_1 = \tau r(C_1)$

$r = K C_1$

$= K_0 e^{-\frac{E}{RT}} C_1$

$T = T_0 + \frac{1}{\lambda} X$

$C_{10} = 2$

$T_0 = 300$

So, now let us try to look at how what happens in a in a reactor in a stirred tank reactor as well as plug flow reactor when we have adiabatic operation. And this is what is what is shown in this particular figure over here when we have when we have non isothermal reactor in a stirred tank stirred tank operation. So, what we have done over here is, we have what we have d 1 is we have once again considered a single reaction and putting some values of and we have our energy mass balance which is in terms of r of C 1 which we just now saw. Let us assume that the reaction is simply first order reaction but remember, our K is dependent on temperature and temperature is dependent on conversion or concentration. And therefore, this relationship is not a linear relationship anymore and we have we have non-linear non-linear relationship.

So, let us look at what happens when we try to change the residence time tau. So, that is what is plotted on the x-axis and how does how does the concentration as well as temperature vary in the in the reactor? There are some numbers that I have taken for this illustration, for example, C 1 0 is taken as 2 and so on. So, for all these K not e, there are some some values assigned to it, but these values are not that important but the behavior of the of the reactor that is that is u H u H important So, what what do we see when the residence time is low or short? For shorter residence time, you expect that there will be very little reaction and therefore, concentration C 1 is very close to the inlet concentration. As we increase the residence time, more reaction takes place and therefore, concentration decreases; however, this decrease in concentration is not monotonic. In fact, the concentration behavior is of this kind. Now, since our concentration is changing in this particular manner, we can write temperature because temperature is related to concentration and therefore, temperature for example, inlet temperature T naught I have taken it as 300.

So, when there is very little reaction temperature in the exit is close to temperature at the inlet. But as we increase the residence time, we have more and more more and more increase in temperature because reaction is reaction is taking place. Remember, here we have exothermic reaction in my when we are looking at this particular reaction. So, now, what happens? Suppose if I have a residence time which is unity? So, at this residence time I have three possible values of concentration; number 1, number 2 and number 3. This behavior once again is similar to what we saw in an non isothermal catalyst reactor behavior that is multiplicity of multiplicity of steady state. What is this multiplicity of steady state? That is, for the same residence time under exactly identical operating conditions, I have three different possible values of steady state concentration and therefore, the temperature as well 1, 2 and 3. What are their characteristics? 1 for example, or let us start with 3 Number 3 for example, the inlet concentration and the reactor exit concentration are almost close to each other; that means, hardly any reaction has taken place. In case of 1, the exit concentration is significantly lower compared to inlet concentration. So, lot of reaction has taken place; the similar behaviour can be seen in the case of temperature also; number 1 So, this is my actually number corresponding to number 3, 2, 1.

So, concentration difference is very high at number 1; that means, conversion is very high. So, temperature is also significantly different than the inlet temperature, number 2 is intermediate but as we had seen previously and we will see little later on that this state is very difficult to difficult to achieve without any control that is in inherently unstable.

So, we will talk about the stability of the reactor and then at that point of time, we will once again visit these number 1, 2, 3 steady state and see see u H what happens.

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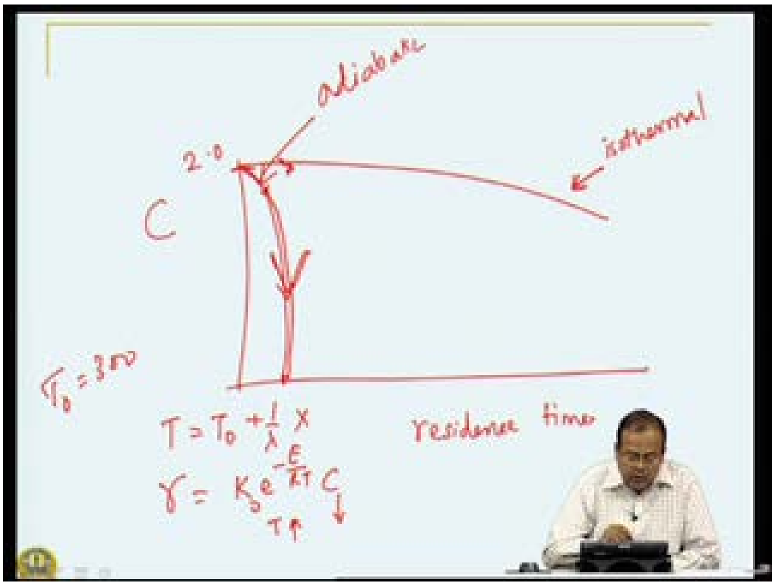

Now, let us let us go back let us let us look at what happens when we have plug flow reactor and for some reason, my diagram is missing but let me let me just let me just plot it the same concentration versus versus residence time. For the same values of these parameters that we had considered, we get a behavior which looks something like this although I do not have exact numbers numbers over here but we have we have reaction occurring very rapidly. So, this is for adiabatic operation and this is what will happen for steady state or isothermal operation. What what we are looking at over here, is a behavior where suppose we said that earlier; we said that we had taken this in inlet concentration as 2 and the temperature was inlet temperature was 300. Suppose, suppose if I carry out a reaction in an isothermal manner by maintaining the temperature temperature at the same value as 300, this is the what behaviour I will get; that is to achieve any appreciable conversion, I have to wait for a long time whereas, the same behaviour in an adiabatic reactor is completely different. In fact, the behaviour is very similar at the starting point because conditions are same. But what happens in a in a in an adiabatic process? In an adiabatic process, as our conversion increases or concentration decreases in exothermic reaction, temperature increases. Now, what happens as temperature increases? Remember, this is our rate.

So, our concentration is decreasing but our temperature is increasing, increase in temperature exponential term with negative E by R T this term increases and rate of reaction increases and therefore, the concentration decreases now much rapid as compared to when temperature was constant. How rapid is this temperature effect? If you look at look at the behaviour over here, the slope is almost infinity, why is that? Because, temperature the rate is highly sensitive to temperature increases. Remember, we talked about it in our first or second class; that is even a ten degree temperature can almost double the rate of reaction. So, as the temperature increases the rate increases, as rate increases concentration decreases, decrease in concentration further increases the temperature leading to almost runaway reaction; that is the consumption of the reactant is almost infinitely fast, if this reaction is to take place in an adiabatic reaction. Now, you will start appreciating what I had said sometime back that why is adiabatic operation important? Remember, here this is almost like an uncontrolled reaction because the slope is almost infinity. So, do you not know what will happen if such situations arise? And therefore, knowledge of adiabatic operation is important; eventually the rate will go to 0 because all reactant has got consumed but before that, the reaction just accelerates to a very large value and we do not know what other effects side effects if at all such behavior may may have.

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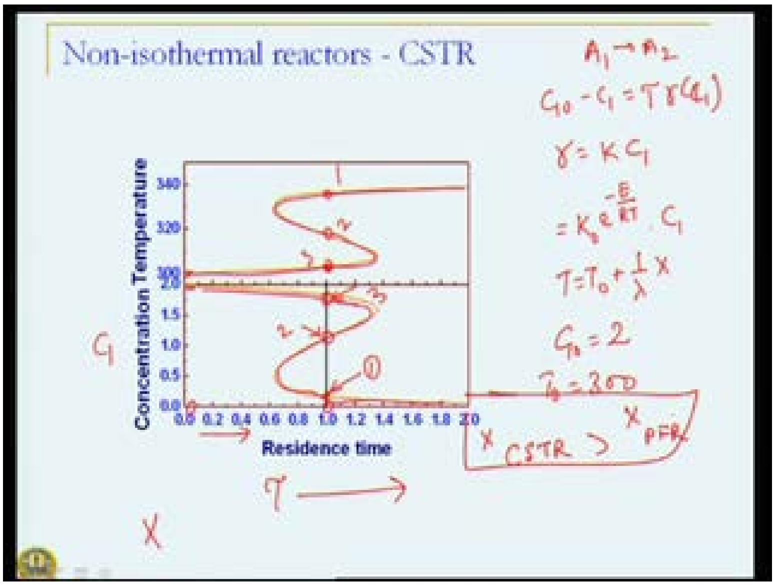

Non-isothermal reactors - CSTR

$A_1 \rightarrow A_2$

$C_{10} - C_1 = \tau r(C_1)$

$r = k C_1$

$= k_0 e^{-\frac{E}{RT}} \cdot C_1$

$T = T_0 + \frac{1}{\lambda} X$

$C_{10} = 2$

$T_0 = 300$

$X_{CSTR} > X_{PFR}$

So, let us try to look at what is happening in this particular scenario. Also, although I do not have I don’t have numbers here. But also it. It happens that the for the same residence time, the conversion in a C S T R now, is much better than conversion in a plug flow reactor. Remember, for an non for an isothermal reactor C S T R always perform poor compared to plug flow reactor because we saw the reason for that in a plug flow reactor, concentration decreases form the entry point to the exit point in a gradual manner. So, the rate of reaction also decreases in a gradual manner and therefore, compared to C S T R. In C S T R, entry to exit drop in concentration is almost instantaneous. Therefore, the reaction rates are very low, where as in a plug flow reactor there is gradual decrease in reaction rate. So, in general reaction rates are higher than C S T R and therefore, we have we have higher rate of rate of reaction in the plug flow reactor. So, better conversions; however, So, this is what happens for non isothermal for an isothermal reactor, for non isothermal reactor the conversion in a C S T R is actually better than the plug flow reactor for non isothermal for isothermal its other way wrong..

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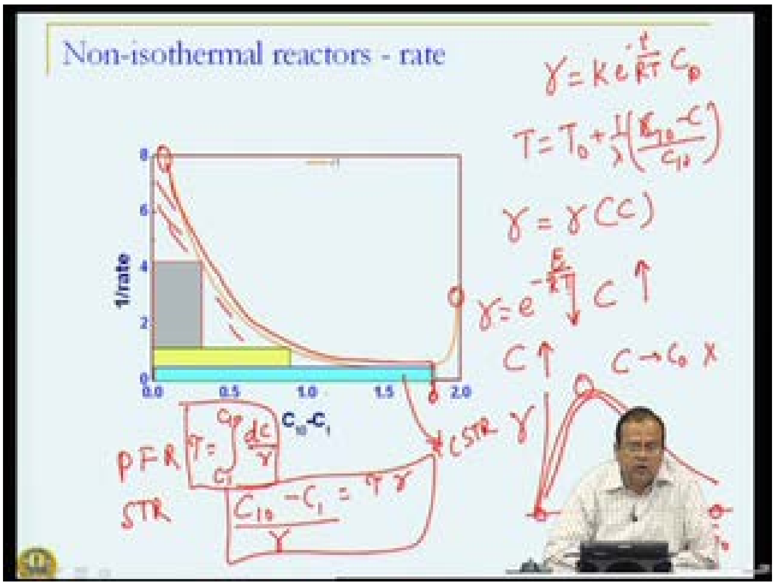

Non-isothermal reactors - rate

So, let us try to look at why is this why this happening? So, let us try to go back to the rate which is exponential E by R T into C and my temperature is related to conversion. So, what happens to the rate as a function of concentration, because we eventually last time few minutes back we wrote this whole thing as a as a function of function of concentration. So, what happens to the rate as a function of concentration? Now, if you look at the rate, there are two important effects. I am not writing the K naught constant? So, as C increases or let us say as C increases this term will increase, but this term will decrease, why? Because higher the value of C R if C is close to C naught X is low. So, temperature is temperature is low.

So, what happens is the rate versus concentration plot actually looks now something like this. Why is this behavior? If concentration is low, the rate is low because it is linearly proportional, if concentration is high. Remember, concentration and temperature are related to each other. So, concentration for example, is close to C 1 0 that is high, temperature is close to inlet temperature which is a low value, so E raised to minus e by R T is a low value and therefore, the product is also low. So, at both low concentrations and high concentrations, the rate is low passing through maxima as concentration is increased. So, as concentration is increased both these will effect will have counter balancing each other and will pass through pass through maxima. So, what does it mean in terms of plot of 1 over rate versus C 1 0 minus C 1? So, when C 1 is close to C 1 0. So, let us say this is my C 1 0, the rate is at a high value when C 1 is close to 0 or the rate is also a low value. So, 1 over R is high and this is this is what gives me my reaction rate 1 over R versus 1 over C.

Now, if you recall, we talked about design equations for plug flow reactor and stirred tank reactor. The design equations are still the same because we have now written what is for stirred tank reactor C 1 0 minus C 1 is tau into r or residence time is C 1 0 minus C 1 by r and for plug flow reactor, it is integral d c by r from C 1 to C 1 0 which is my residence time or in other words graphically for plug flow reactor residence time is area under the curve for stirred tank reactor it is the area of the area of the rectangle. So, let us let us look at what happens and we talked about how we can relate it to 1 over rate versus C 1 0 minus C 1 plot. So, what happens for example, my C 1 is a small value. So, somewhere over here the blue rectangular area is the conversion that we will get or that is is the residence time that is required to achieve that conversion. So, this is my C S T R tau C S T R and what will be what will be the area for for plug flow reactor? It will be the area under this 1 over r versus C 1 0 minus C 1 curve.

So, this entire entire area which is certainly is much greater than that for a stirred tank reactor or in other words, for a non-isothermal reactor adiabatic reactor, the residence time required in a stirred tank reactor to achieve certain conversion is much smaller than the residence time required in a plug flow plug flow reactor. So, this is different from isothermal reactor so. In fact, what we have made use of, in an adiabatic reactor since temperature increases for exothermic reaction that increase in temperature results in increasing of rates and therefore, the residence time is is smaller for C S T R, for the same reason in a C S T R, increase in temperature will be instantaneous. So, the reaction rate will go to a high value almost instantaneously whereas, in a plug flow reactor, the increase in temperature will be gradual. So, increase in rate will be gradual. So, as a result, stirred tank reactor the residence time will be much shorter than the plug flow plug flow reactor. Now, let us look at what do we what happens when we have reversible reactions, that is, what is the behavior for reversible reaction again in an isothermal or non-isothermal situation?

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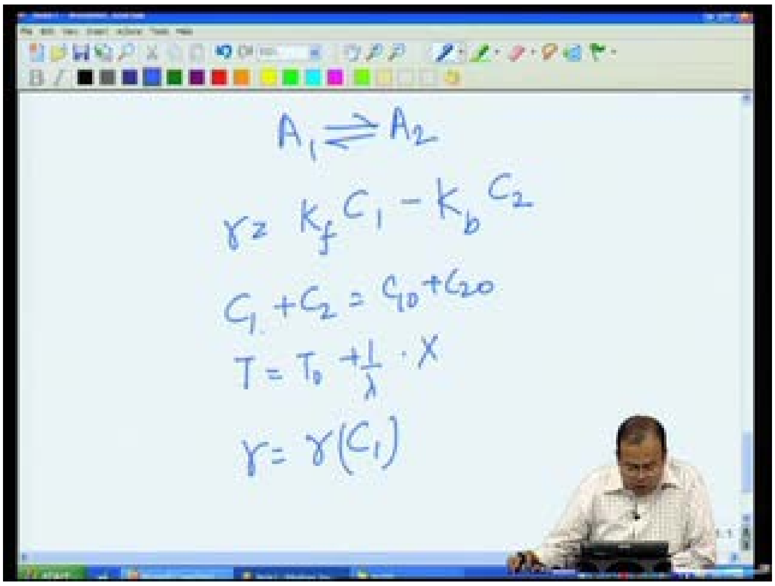

$$A_1 \rightleftharpoons A_2$$

$$r = k_f C_1 - k_b C_2$$

$$C_1 + C_2 = C_{10} + C_{20}$$

$$T = T_0 + \frac{1}{\lambda} \cdot X$$

$$r = r(C_1)$$

So, our energy balances are same as before, but we have to now remember that we are looking at a reversible reaction or in other words let us say, our reaction is A 1 going to going to A 2.. So, our rate of reaction is forward reaction rate constant into concentration of C 1 minus backward reaction rate constant into concentration of C 2. We know C 1 and C 2 are related to each other that is C 1 for example, plus C 2 must be C 1 0 plus C 2 0; overall mass balance equation. Now, temperature and concentration are also related to each other why because if you look at these relationship between stirred tank reactor and so on, when we looked at mass and energy balance and it is coupling. We never specified what R is, it could be first order reaction, it could be reversible reaction; if reversible reaction we just considered a single reaction and coupled this two.

So, this coupling must also be valid when we have a reversible reaction or or in other words we have we have this 2 this two kinds of kind of relationship that is T is equal to T 0 1 over lambda into X. So, we have C 2 related to C 1, we have temperature related to C 1 or in other words, we still can write these reaction rate as a function of concentration or as a function of temperature or as a function of function of conversion. So, let us look at what happens what happens when we have when we have this particular reaction.

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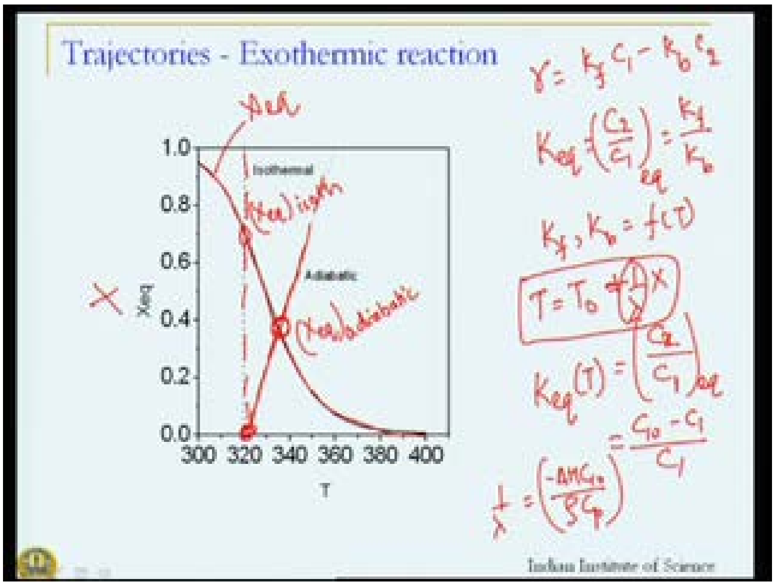

Trajectories - Exothermic reaction

$r = k_f C_1 - k_b C_2$

$K_{eq} = \left(\frac{C_2}{C_1}\right)_{eq} = \frac{k_f}{k_b}$

$k_f, k_b = f(T)$

$\boxed{T = T_0 + \frac{1}{\lambda} X}$

$K_{eq}(T) = \left(\frac{C_2}{C_1}\right)_{eq} = \frac{C_{10} - C_1}{C_1}$

$\frac{1}{\lambda} = \left(\frac{-\Delta H C_{10}}{\rho C_p}\right)$

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So, what we are looking at over here is for a reversible reaction for a reversible reaction. So, K f into C 1 minus K backward into C 2; K f and K backward are functions of temperature. But we also know that we have K equilibrium defined from thermodynamics which is K f by K b right which is nothing but C 2 by C 1. So, at equilibrium the rate of rate of reaction is reaction is 0. So, let me rewrite for we have K equilibrium which is C 2 by C 1 at equilibrium which is K f by K b. We also have K f K b which are functions of temperature and for an adiabatic operation, we have lambda into lambda into x. So, suppose we now plot conversion as a function of temperature we have for example, our equilibrium line right this is what we have seen earlier. For an exothermic reaction, the equilibrium conversion decreases as temperature is increased. So, we have we have this particular particular line.

Now, what happens when we do an isothermal operation? So, let us say that we are doing an isothermal operation at this particular particular condition. So, what we are plotting here, in general is x versus T and this is specific case of x equilibrium. How do we get that x equilibrium? Because we know K equilibrium, which is a function of temperature, which is C 1 sorry C 2 by C 1 at equilibrium and let us say that we do not have any C 2 0. C 2 is nothing but C 1 0 minus C 1 divided by C 1. So, we have a relationship between temperature and equilibrium conversion and this is what this is what we we get.

Now, what happens when you have a isothermal operation? When you have a isothermal operation, temperature is constant. So, this is my isothermal is othermal operation. So, in an isothermal operation my conversion will keep on increasing till I reach the equilibrium limit and that is the maximum conversion I will get. now Let us say that we have an adiabatic operation, exothermic reaction now, what happens for an adiabatic operation from this particular relationship? We see that relationship is linear right between between conversion X and temperature T and we also know this constant 1 over lambda what is 1 over lambda is minus delta H C 1 0 by rho C p. So, if exothermic reaction delta H is negative. So, minus delta H is positive. So, 1 over lambda is lambda is positive or in other words, for adiabatic reaction X versus T is a straight line with a positive positive slope. So, what will happen if you start the same reaction, same temperature,, but it is in an adiabatic manner? The temperature will increase temperature will increase and it will eventually we will reach equilibrium. So, this is X equilibrium for isothermal operation; this is the equilibrium limit for adiabatic operation. Now what has happened? The maximum conversion in an adiabatic reactor will be lower than the maximum conversion in an isothermal reactor. It is not a not a situation that we would like to be because what it means if the equilibrium conversion is low, that is the maximum you can get. So, the actual you will get will be much lower than that. So, adiabatic operation from thermodynamic point of view is not a favorable operation, isothermal operation on the other hand is, but what happens to the kinetics? Thermodynamics is only one part of our whole scheme of things. So, what happens to kinetics? Now, kinetics if you see temperature is constant.

So, in general the rate of reaction will be low. So, here the temperature is increasing if you are travelling along the adiabatic path; that means, the reaction rate is now increasing. So, we will reach the equilibrium conditions much faster compared to isothermal. So, the kinetics is favorable on an adiabatic path but the thermodynamics is not, whereas, on an isothermal reactor operation, kinetics is unfavorable whereas, the thermodynamics or equilibrium is favorable. So, in both these conditions, both these extremes, we are not in a happy situation either way, it is always give and take. In isothermal case, what you gain by thermodynamic way, that is a maximum conversion you lose in a kinetic sense whereas, in an adiabatic reactor, you gain on a kinetic sense but lose on the thermodynamics sense. So, how should we operate these how should we operate these operate these reactors? So, clearly operating either as a isothermal reactor or as a adiabatic reactor is not an ideal scenario, we have to find a combination of these two cases..

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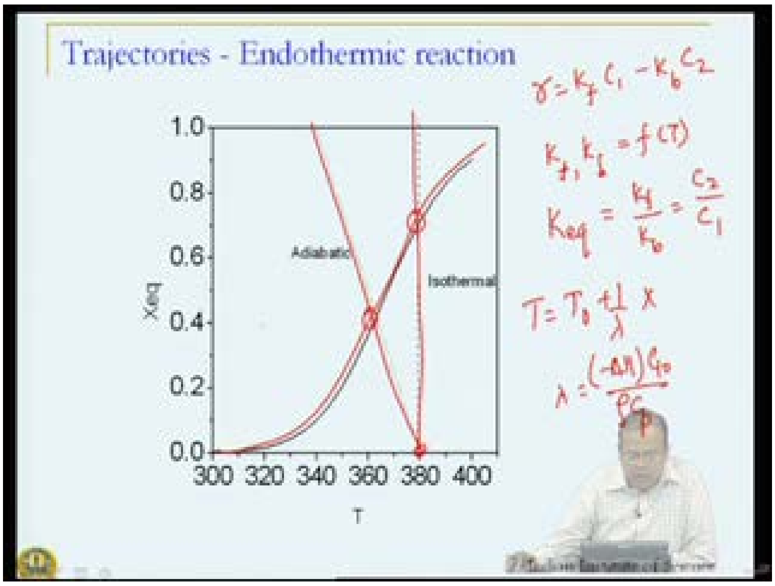

Trajectories - Endothermic reaction

$r = k_f C_1 - k_b C_2$

$k_f, k_b = f(T)$

$K_{eq} = \frac{k_f}{k_b} = \frac{C_2}{C_1}$

$T = T_0 + \frac{1}{\lambda} X$

$\lambda = \frac{(-\Delta H) C_{10}}{\rho C_p}$

So, how do we go about do that? but before we do that, let us look at what happens in an endothermic reaction. In an endothermic reaction, reversible the same, now our equilibrium conversion increases as temperature is temperature is increased but temperature relationship with conversion where lambda is minus delta H C 1 0 by rho C p, what happens to delta H positive endothermic reaction. So, lambda is negative. So, this is my adiabatic line, this is my isothermal isothermal line. So, what happens here, if I carry out this isothermally with this particular temperature? My equilibrium conversion will be also high and temperature is also high whereas, for an adiabatic process my equilibrium conversion is low and temperature is also low because what is happening adiabatic endothermic reaction means energy will be removed from the system. So, temperatures will be lower. So, both in a kinetic sense as well as in a thermodynamic sense, adiabatic operation is not desirable whereas, isothermal operation is desirable both from kinetic and thermodynamic sense but to maintain isothermal conditions for an endothermic reaction, you will have to supply energy. Otherwise, by itself temperature will go down. So, that is the price that we may have to we may have to pay, but coming back to exothermic reactions, we saw that we have to strike a balance between adiabatic operation and isothermal operation and we will look how this balance is achieved little later on.

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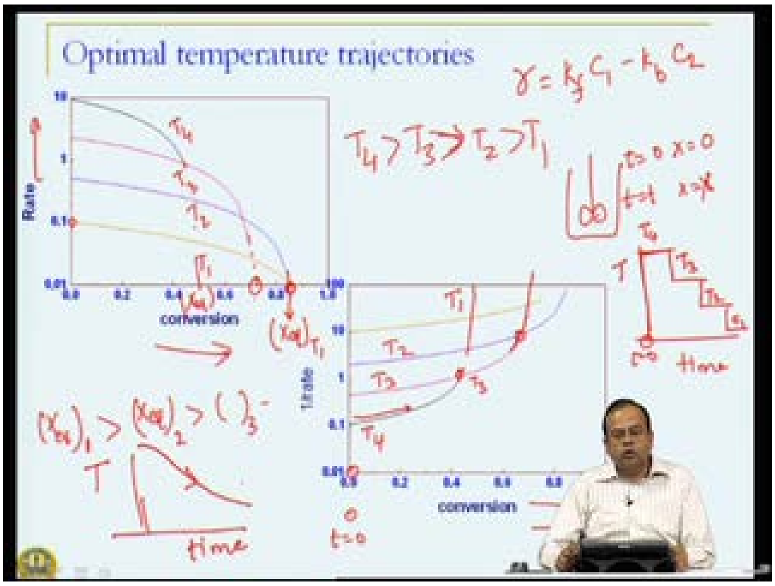

Optimal temperature trajectories

But, but let us look at look at how do we how do we operate these operate these reactors. For example, remember rate C 2, that is one idea and in an exothermic reaction, what happens to the happens to the rate as we increase the increase the temperature? So, what we are seeing here is conversion on the x-axis and rate on the y-axis. So, let us say that we start with temperature some temperature T 1, a low temperature. So, our as we are increasing the conversion, the rate will go to 0 and this is my equilibrium conversion at temperature T 1 as I increase my temperature. So, these are my T 1, T 2, T 3, T 4 saying T 4 greater than T 3 greater than greater than T 2 greater than T 1. So, what is happening as I as I am I am increasing my temperature? For example, T 3 this is what will my equilibrium conversion will be for T 3, this will be for T 2 and so on.

So, what happens to my equilibrium conversion? X equilibrium conversion for temperature T 1 is greater than same thing for 2 3 and so on, because my temperature, that is my characteristic of my exothermic exothermic reaction but what is happening to the rate? The rate is higher at temperature T 2 because of erroneous affect same as T 3 T 4. So, if we now plot 1 over r versus conversion because remember that is what determines my performance in a in a reactor. So, how does 1 over R at lower temperature? This will be the highest value 1 over are because r is low then the followed by T 2, followed by T 3, followed by T 4 and so on. So, now, what will happen as the reaction is reaction is taking place? So, let us say that we are try ing to operate a batch reactor, let us consider a simple simple scenario of batch reactor. So, we are now trying to see what should be my temperature for a batch reactor which is handling an exothermic reversible reaction, which gives me the lowest residence time to achieve some desired conversion? We know, the lowest residence time will be obtained when the rates are high or in other words, if you look at 1 over rate; when 1 over rate is low.

So, now, imagine this is my batch process stirred tank reactor batch process at time T equal to 0, conversion is 0 and at time T equal to sometime T conversion is x. So, I start. So, this is my conversion 0 and then I am increasing the conversion, so this is equivalent to time being 0 and time increasing, so what happens? When the conversion is low, 1 over r is lowest with the temperature T 4. So, let me let me just plot on the side; time and what is it what temperature gives me highest rate or lowest 1 over rate. So, at the start T equal to 0 highest temperature gives with the lowest 1 over r; that means, at the start my temperature should be T 4. ok

Suppose I keep the temperature T 4 for very long time, what will happen? If you look at over here as conversion is increasing, I am hitting the equilibrium limit. So, if I keep temperature T 4 for a long time, I will reach reaction rate equal to 0 or this line will now go like this; that means, I have lost now on equilibrium conversion if I keep temperature T 4 for a long time. So, suppose it crosses over here, what should I now do now? I see now that temperature T 3 is what is giving me the lowest lowest rate or in other words, I should decrease my temperature to T 3. But that again I cannot keep that forever because at some point, this line also crosses. So, after this point, I see my T 2 temperature gives me lower 1 over r; that means, I should reduce my temperature to T 2, further reduce it to T 1 and so on.

So, what should I how should I operate my batch reactor for reversible exothermic reaction? If I am trying to do it in a non isothermal manner, keep high temperature initially, then lower the temperature lower the temperature further. lower the temperature. So, what what is the idea now? Initially, we are nowhere near equilibrium. So, high temperature gives advantage of kinetics and we are still not restricted by thermodynamics, but if you keep this temperature high for a long time, your equilibrium value equilibrium conditions will be achieved and equilibrium conversion at high temperature is low. So, you shift to a lower temperature T 3 and keep doing this so that you get best of both kinetics as well as thermodynamics. Suppose I were to do it in a step wise manner, but I can now extend this saying that for an exothermic reaction in a batch reactor, my temperature should increase or rather decrease from a high value to a low value as reaction proceeds. The counter part of this in a plug flow reactor is my temperature should decrease along the length of the reactor. How do we do that? We will try to see in subsequent subsequent classes, so, we will stop here for the day.