# Advanced chemical Reaction Engineering

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## Lecture - 18

## Energy balance - III Design for Constant T Operation

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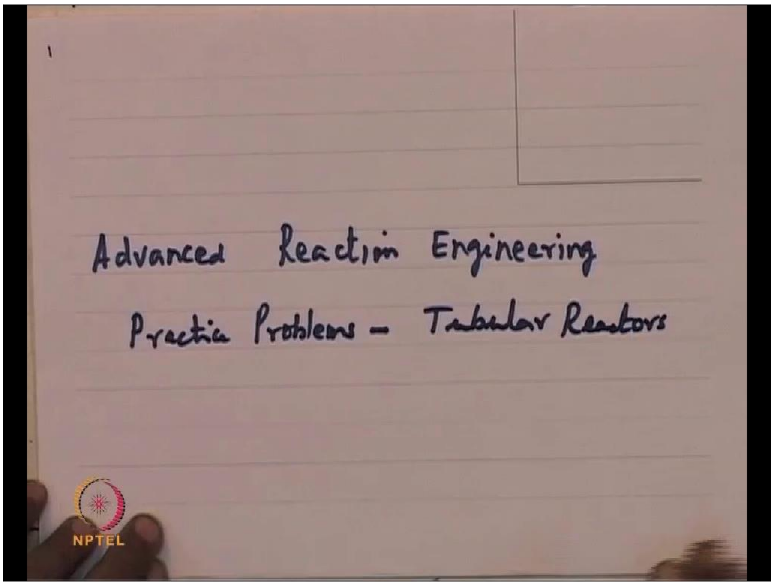

Advanced Reaction Engineering

Practice Problems - Tubular Reactors

Look at advance reaction engineering. Today, we look at practice problems; look at tubular reactors. This is the exercise for today. We all know that tubular reactors are very common in the process industry.

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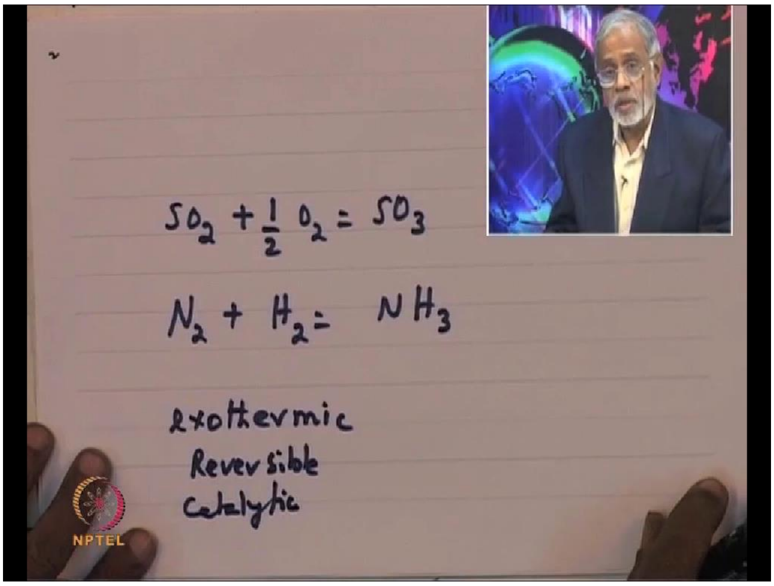

$SO_2 + \frac{1}{2} O_2 = SO_3$

$N_2 + H_2 = NH_3$

exothermic
Reversible
Catalytic

Fine examples of that would be sulphur di oxide plus oxygen, giving you sulphur tri oxide. Then, you have nitrogen plus hydrogen, giving you ammonia. These are finest examples of exothermic reversible. These are all exothermic reversible and catalytic. They all require catalyst. Examples that our process industry uses, extensively; we want to look at some of these to understand some of the intricate details, going to it and some strategies that help us to understand to how to manage these reactions in the process industry. Now, to put it in the context, let us take an example.

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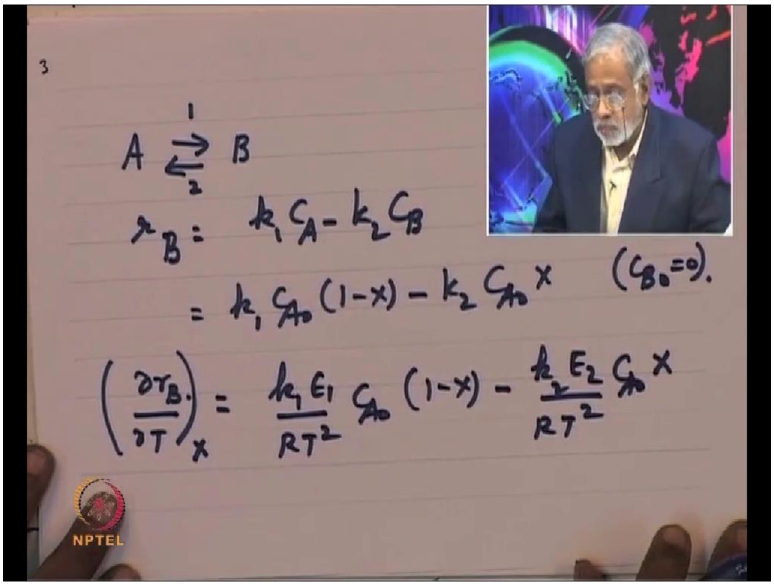

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$$A \underset{2}{\overset{1}{\rightleftarrows}} B$$

$$r_B = k_1 C_A - k_2 C_B$$

$$= k_1 C_{A0}(1-x) - k_2 C_{A0} x \quad (C_{B0}=0).$$

$$\left(\frac{\partial r_B}{\partial T}\right)_x = \frac{k_1 E_1}{RT^2} C_{A0}(1-x) - \frac{k_2 E_2}{RT^2} C_{A0} x$$

Let us take an example; A going to B; 1, 2, a reversible reaction. Let us say, let r b equal to k 1 C a minus of k 2 C b as an example; not to illustrate how things would happen. So, this is k 1 C a 0, 1 minus of x, minus of k 2 C a 0 times of x, of course, assuming that C b 0 equal to 0. Frequently, this would be the case that applies. Now, if we look carefully at this reaction, we find that this term, del r b by del t at constant x; what is del r b by del t at constant x? You need to differentiate this one. We will get k 1 E 1 by r t square C a 0 times 1 minus of x, minus k 2 E 2 by r t squared C a 0 times of x. Now, it is known that for each x, this r b goes to maxima. On other words, if we said it is equal to 0, we get an equation, which is x m by 1 minus of x m, equal to k 1 by k 2, E 1 by E 2. What is k 1 by k 2; it is equilibrium constant, times E 1 by E 2. So, what we are saying?

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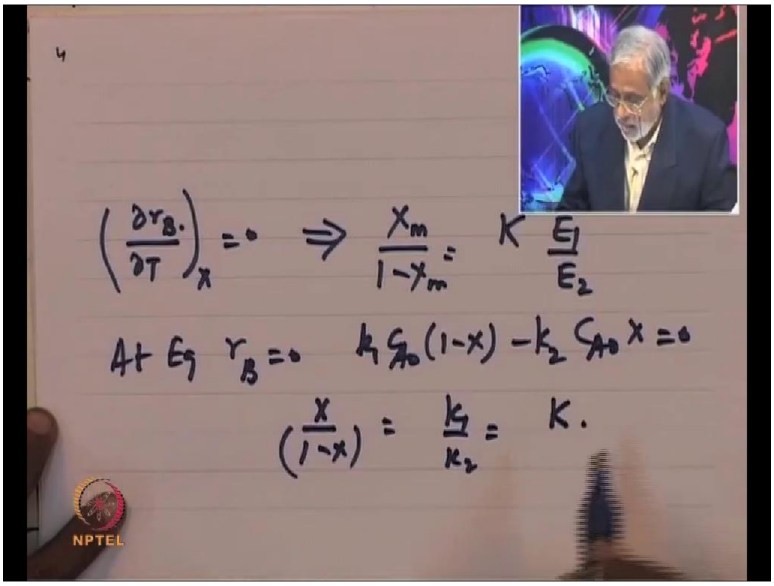

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$$\left(\frac{\partial r_B}{\partial T}\right)_x = 0 \Rightarrow \frac{x_m}{1-x_m} = K\frac{E_1}{E_2}$$

At Eq $r_B = 0$ $\quad k_1 C_{A0}(1-x) - k_2 C_{A0}\, x = 0$

$$\frac{x}{(1-x)} = \frac{k_1}{k_2} = K.$$

What we are saying is that that del r b by del t at constant x goes to 0. This implies x m by 1 minus of x m, equal to k equilibrium constant time E 1 by E 2. Now, if we look at this reaction, this reaction at equilibrium r b equal to 0. So, at equilibrium r b equal to 0, which means that k 1 C a, 1 minus of x, minus of k 2 C a times x equal to 0, which means that x by 1 minus of x equal to k 1 by k 2, equal to k. Notice that x m by 1 minus of x m is k times of E 1 by E 2 and at equilibrium, I will call it here; this is at equilibrium. I should put x c here;, so x c by 1 minus x c equal to k. So, the forms are very similar and we have already shown this. So, there is no need to go through this, once again. We have shown that plots for an exothermic reversible reaction.

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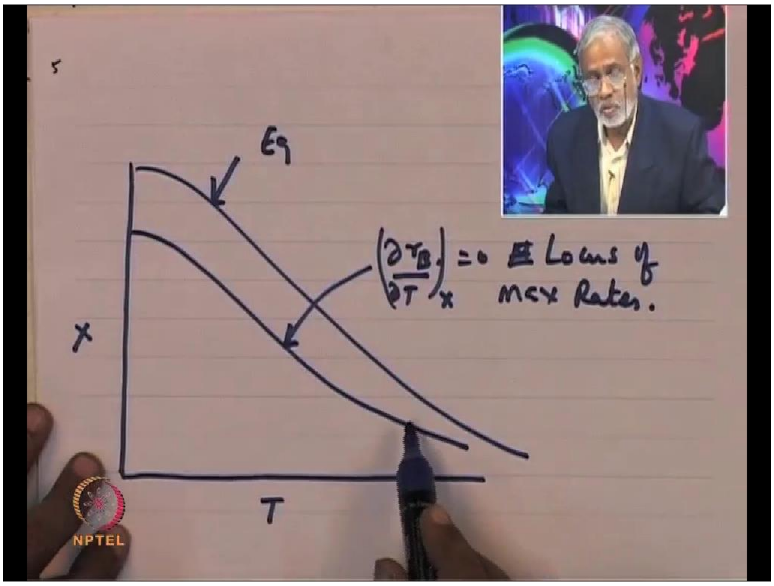

If you make a plot of t versus x, if you make a plot, the equilibrium; this is the equilibrium curve; which means, this curve is described by this equation. Now, if we make a plot of this equation, x m by 1 minus x m k E 1 by E 2, this curve will look something like this. This is, I will call it as del r b by del t at constant x equal to 0 or we can call it as locus of max rates. Now, why are we doing this? We are doing this to understand how to conduct this reaction in a tubular reactor. So, that is, essentially, what we have done is we have found out the locus of maxima in reaction rates; that is appropriate to this reaction. So, clearly, if you want to have a good design, you would like to see that our process runs along this line, so that, the size of the equipment would be as small as possible.

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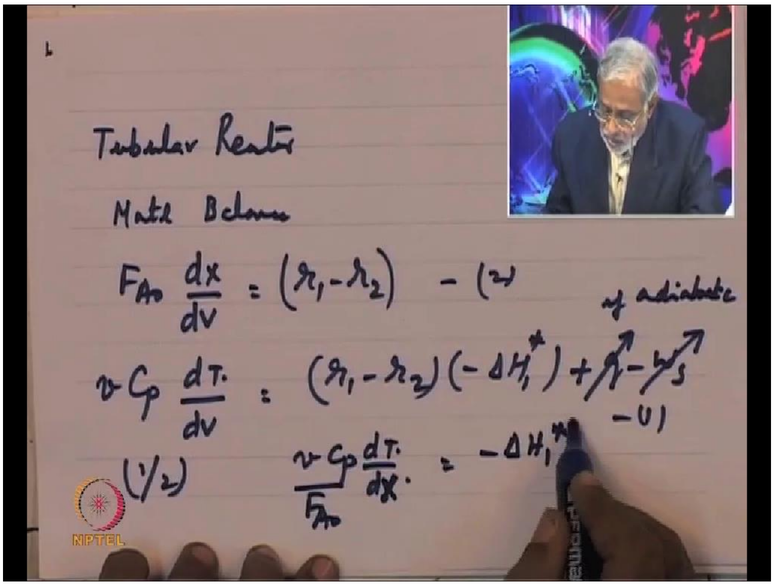

Tubular Reactor

Matl Balance

$F_{A0} \frac{dx}{dv} = (r_1 - r_2)$ – (2)

q adiabatic

$v C_p \frac{dT}{dv} = (r_1 - r_2)(-\Delta H_1^*) + \cancel{q} - \cancel{w_s}$ – (1)

(1/2) $\frac{v C_p}{F_{A0}} \frac{dT}{dx} = -\Delta H_1^*$

Let us say we have a tubular reactor; that means, look at a tubular reactor. What is our tubular reactor design equation, our material balance? Our material balance will look like F a 0 times d x d v equal to r 1 minus of r 2; this is material balance. Our energy balance look like this; d t d v equal to r 1 minus of r 2 times, minus of delta H 1 star, which is the heat of reaction, plus q minus of w s. We said we do not look for any work from the system and if it is adiabatic; let us look at the moment, the situation of a tubular reactor, material balance and energy balance under adiabatic situation; that means, we do not allow heat to go out of the system. Now, if I call this as equation 2, and if I call this as equation 1, if I do 1 divided by 2, we will get v c p, d t d v, divided by d x d v. So, I will call this is d t d x; this is F a 0; r 1 minus r 2 cancels off. So, we are left with minus of delta H 1 star. Just checks up once again. So, I am just rewriting this equation once again. So, we get v c p. So, this one is a tubular reactor.

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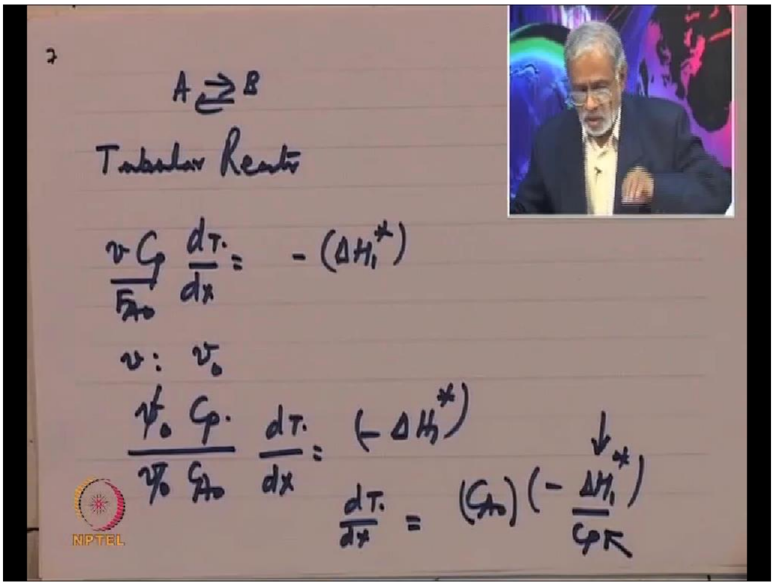

$A \rightleftarrows B$

Tubular Reactor

$$\frac{v C_p}{F_{A0}} \frac{dT}{dx} = -(\Delta H_1^*)$$

$$v = v_0$$

$$\frac{\cancel{v_0} C_p}{\cancel{v_0} C_{A0}} \frac{dT}{dx} = (-\Delta H_1^*)$$

$$\frac{dT}{dx} = (C_{A0})\left(-\frac{\overset{\downarrow}{\Delta H_1^*}}{C_p}\right)$$

We have v times C p; d t times d x; that is left hand side and the right hand side got minus delta H 1 star, equal to minus of delta H 1 star. Now, v, the volumetric flow; in a given reaction, volumetric flow actually, depends on so many factors, particularly, the temperature and so on. If there is change in moles also, volumetric flow will change and so on. Suppose we consider the situation as in this particular case, A going to B and B going to A; v equal to v naught. So, that in this case; F a 0;, so that if I put v equal to v naught, this becomes v naught C p; F a 0 is v naught C a naught d t d x, equal to minus of delta H 1 star or d t d x equal to cancels off. So, it becomes C a 0 times, minus of delta H 1 star, divided by C p. Now, the point of putting it in this form is that, what we trying to say here is that in a tubular reactor, variation of temperature with conversion depends, equal to C a 0, which is a constant. Delta H 1 star by C p; this is typically, not a very strong function of temperature or any other compositions. Similarly, C p, the volumetric specific heat that we have said, is not a very strong function of what happens during the chemical reaction.

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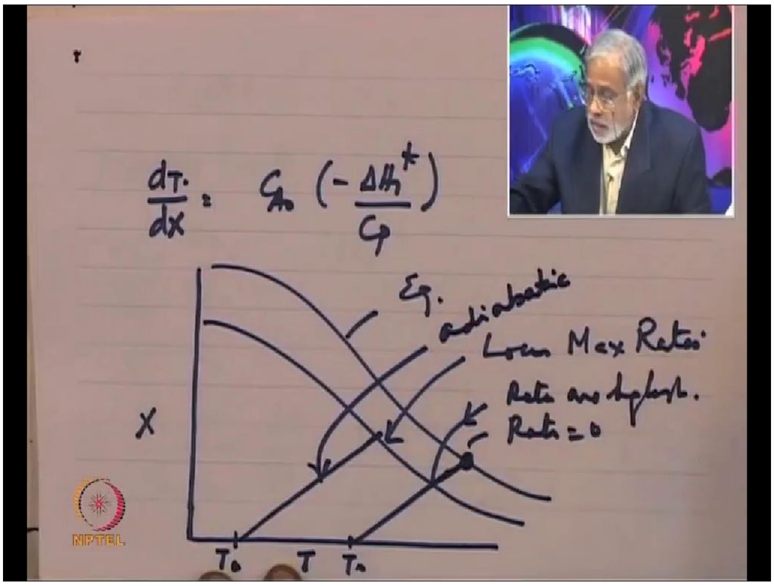

On other words, what we are trying to say is that d t d x equal to C a 0, which is a constant, minus delta H 1 star, which does not change very much; C p also does not change very much. Therefore, the right hand side is the constant. This is the point we are trying to put across. So, right hand side is the constant, if you can see. So, as a result, when you make a plot of x versus t, and you have this equilibrium curve; you have this maxima in rate; this is equilibrium; this is locus of max rates. If our temperature t 0; we are starting it here; as per this equation here, we should expect that we will move along a line, like this or if your t 0 is here, then we will move along a line like this. It will go and touch the equilibrium curve.

At this point, the reaction rates are 0; rates equal to 0. At this point the rates are highest. So, you notice here, as you move along this line with this line is an adiabatic line, as you said; this is the adiabatic line. Why is that adiabatic line? We have knocked out the term q from our equations, because we are writing the equations for the case of an adiabatic process. So, as you move along the adiabatic line, from this point to this point, the reaction keeps on increasing. Here, it becomes maximum. As it moves from here towards the equilibrium curve, the rate keeps on decreasing and become 0 as it touches the equilibrium curve. Now, the question that you and I would like to know is in our design, what do we do? How do we achieve a design which, ensures that the reaction goes; see, this is x. So, we want to go at a higher level of x as possible; that means, you want this to reach this highest value.

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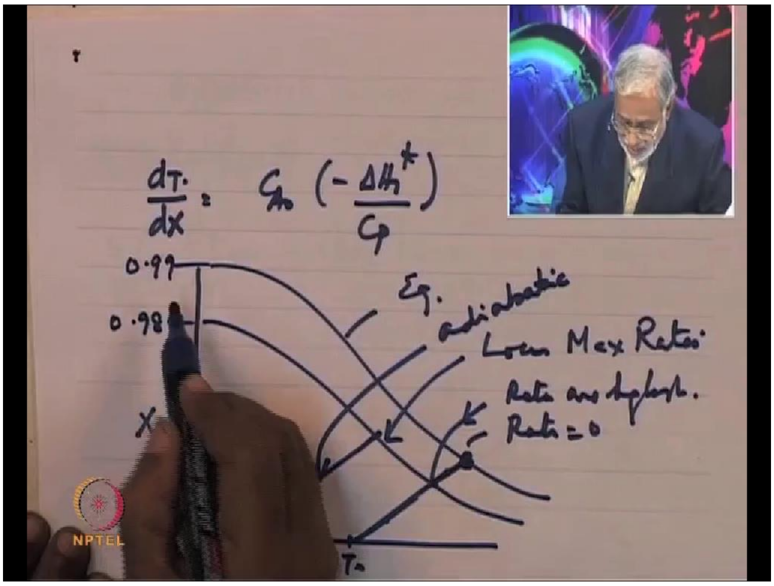

$$\frac{dT}{dx} = C_{A0}\left(\frac{-\Delta H^*}{C_p}\right)$$

Now, if I say this is, in the sense, this is 1; this is 0.99; this is 0.98; let us say and we want to go to as high a conversion as possible; how do we achieve this? Now, what our equations are telling us? What our equations are telling us is that in adiabatic processes, temperature and conversion will move along this line, and then will go and hit the point of equilibria and stop. So, clearly, if this point, the conversion corresponding to this point, this value of x; let us say is 0.3, then clearly, we are not able to reach as high a conversion as you and I would like to reach. Our point in this practice exercise is how do we go to higher and higher levels of reactions; levels of extents of reactions. That is what we would like to do. Let us see how to achieve this.

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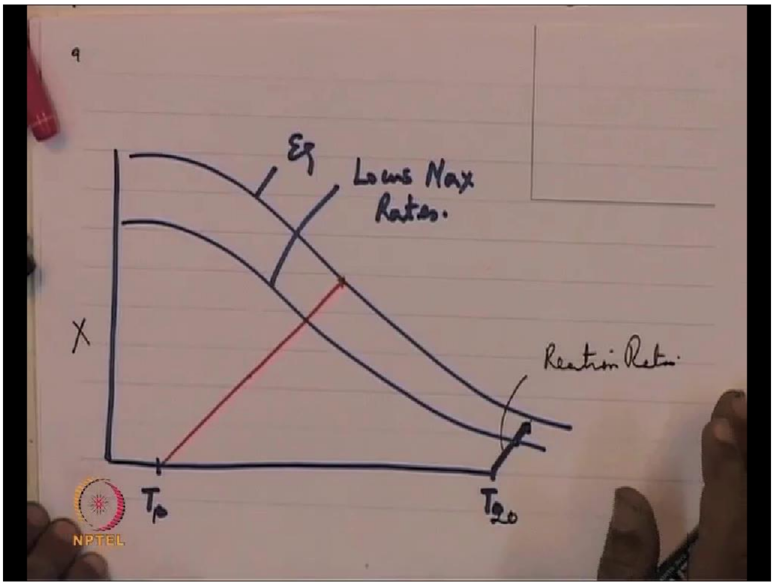

We achieve this by recognizing the following; you have equilibrium curve; you have maximum rate curve; this is the equilibria; this is locus max rates and let us say our feed is available at T naught. Now, if feed is available at T naught, and if you are going to do an adiabatic process, you would probably, travel along this line, and then go and stop there. Instead, if we are heated up this T naught, gone up to this point, T naught here, then once again, this line is able to give you the average reaction rates here. These reaction rates are much larger. Why are they much larger, because the temperatures are much larger. From T 1 0 to T 2 0, what we have achieved is that we have achieved much higher reaction rates, and we are able to move along this curve. Once again, we face the same problem that we have to stop somewhere, because the reaction rate from this point, starts decreasing. So, we would start somewhere here, and then we will start wondering, what is that we must do.

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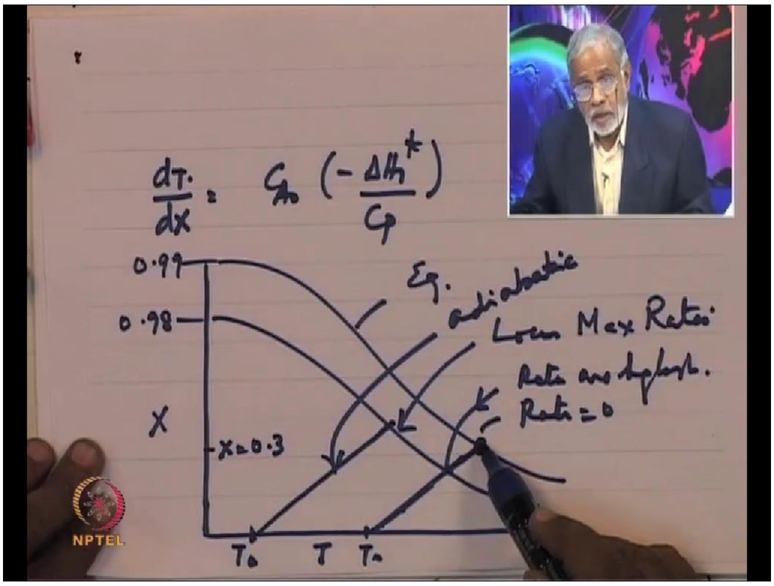

So, what are we trying to say is the following that our tubular reactor equation says that d t d x on the right hand side is the constant, and therefore, the d t d x being the constant, is a straight line and this straight line, if you move along from T 0; if you move along, you can keep going along or you can keep going along up to the equilibria. The moment you reach the equilibria, the reaction rates are nil. At the point of corresponding to this maximum the reaction, the rates are highest. So, as you go from this point to this point, rates keep increasing, and from this point onwards, the rate starts to keep decreasing. When you reach the end point, the reaction stops.

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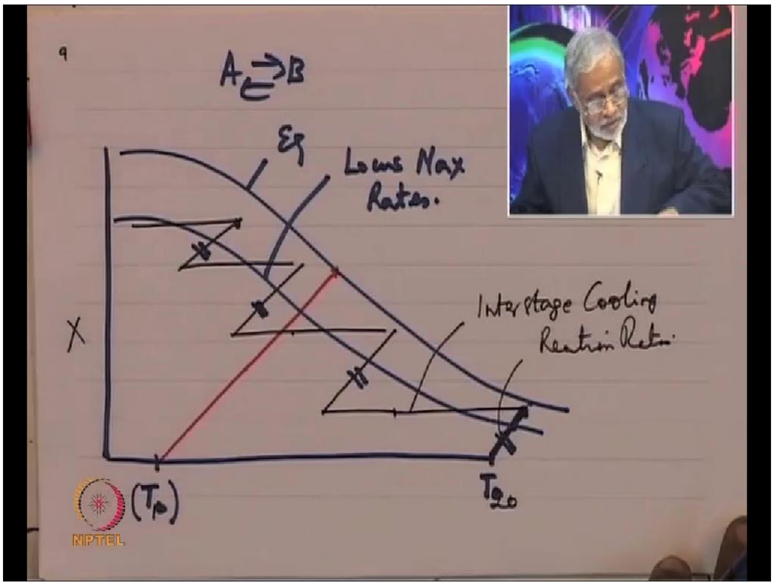

The question is how is it that you and i can conduct this process, so that, we go to the highest level of conversion possible? Now, we notice that if this feed temperature is low, the reaction rates are low. So, that we can pre heat it, and take it up to T 2 0 as the initial temperature, entering the equipment, and then we run an adiabatic reactor. Once again, we will face the same problem that as it approaches the equilibria, the rate becomes very low. You have to stop here. Therefore, how do we go forward from here; too much higher level of conversion for which, what we decide? We run inter stage cooling. So, if we can inter stage cool this, and then once again, from here, we can run one adiabatic reactor.

Once again, we can cool interstage, and then run another adiabatic reactor. We can cool inter stage, and then run another adiabatic reactor, and cool inter stage. On other words, what we are trying to say is that interstage cooling is essential to be able to reach high levels of conversion for reversible exothermic reactions. So, this is this. If we look at sulphur di oxide or if we look at ammonia, you will find that this is reactor 1, reactor 2, reactor 3, reactor 4. So, this is an instance of a 4 stage process where, we go from 0 conversion to a much higher level of conversion. So, this is the exercise that we want to illustrate, and then the numbers are given below.

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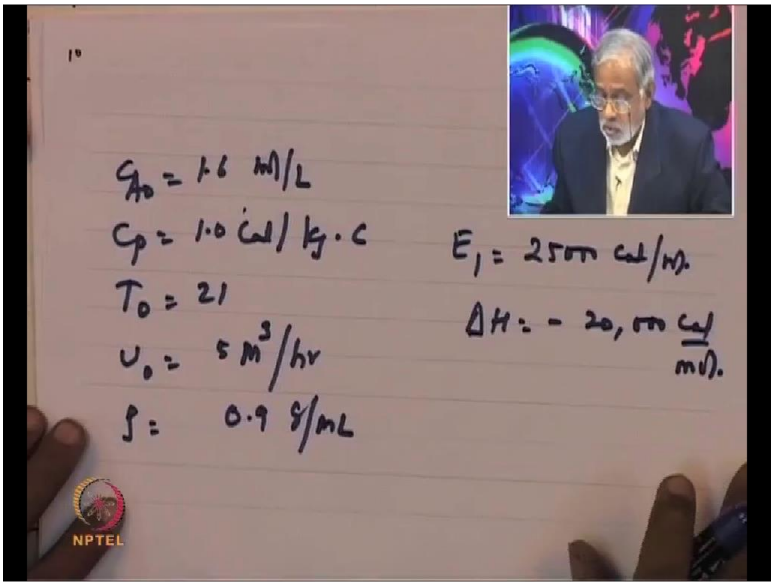

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$C_{A0} = 1.6$ mol/L

$C_p = 1.0$ cal/kg·C

$T_0 = 21$

$v_0 = 5\ m^3/hr$

$\rho = 0.9$ g/mL

$E_1 = 25000$ cal/mol

$\Delta H = -20,000\ \frac{cal}{mol}$

We have a chemical reaction. We have an instance; the data is given here; C a 0 is given as 1.6; specific heat is given as 1.0; this is mole per litre, and then it is calories per kg per c; T naught is given as 21; v naught is given as 5 cubic meters per hour; density is given as 0.91 grams per ml, and then you have E 1, is given as 25000 calories per mole; delta H is given as minus 20000 calories per mole. On other words, the E 1 is known. How is E 2?

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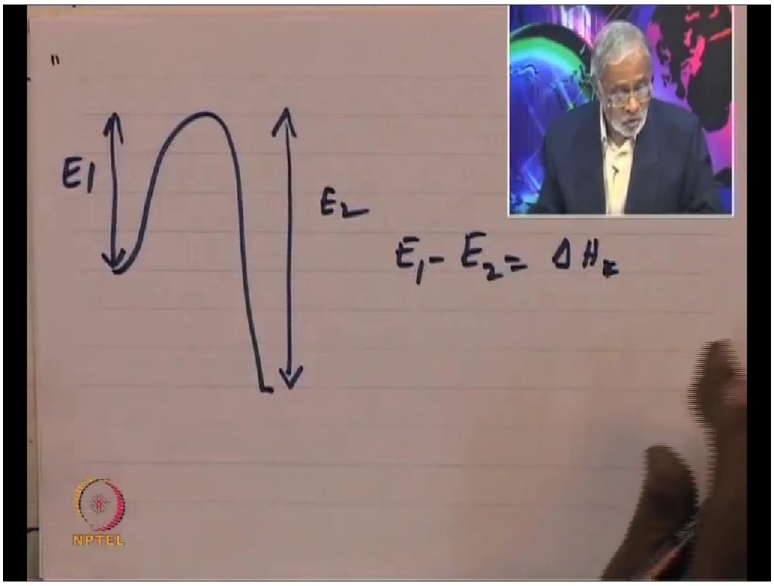

We know that E 1 and E 2 are related by our understanding of basics if you have a chemical reaction which is reversible. So, this is E 2; this is E 2 and this is E 1, and by definition, E 1 minus of E 2 equal to delta H. For an exothermic reaction, E 2 is greater than E 1 and therefore, delta H is negative.

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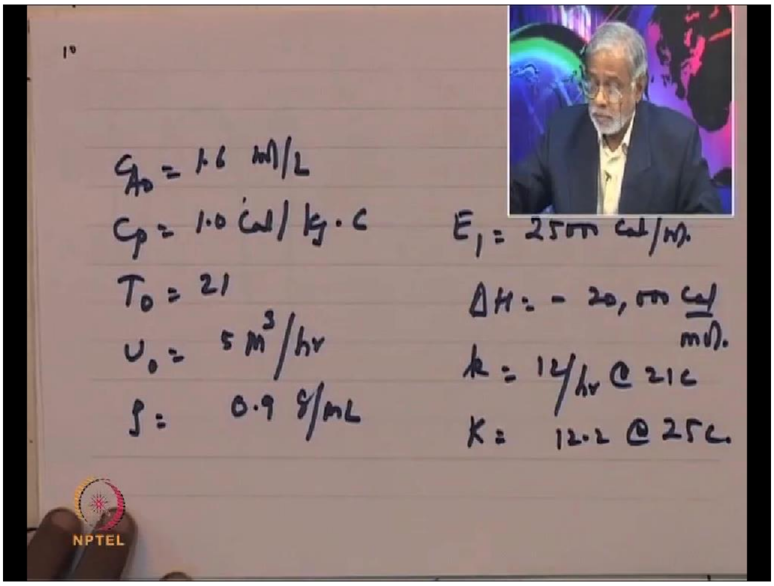

$C_{A0} = 1.6$ mol/L

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$T_0 = 21$

$v_0 = 5\ m^3/hr$

$\rho = 0.9$ g/mL

$E_1 = 25000$ cal/mol.

$\Delta H = -20,000$ cal/mol.

$k = 12/hr$ @ 21c

$K = 12.2$ @ 25c.

If all the data are given below and the rate constant; rate constant k is given as 12 per hour at 21 c. Equilibrium constant is given as 12.2 at 25 c. So, you can see here, rate constants are given; equilibrium constant is given. Therefore, we can plot the equilibrium curve. We know, we can do the whole exercise quickly, so that, we have a good understanding of how the whole things are done for a multi stage tubular reactor design. Let us quickly, run through this for the numbers.

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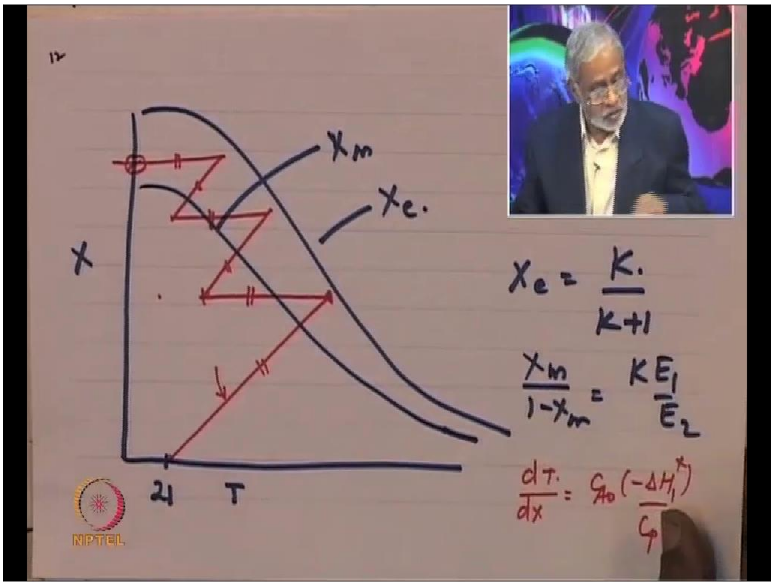

$X_e = \frac{K.}{K+1}$

$\frac{X_m}{1-X_m} = K\frac{E_1}{E_2}$

$\frac{dT.}{dX} = \frac{C_{A0}(-\Delta H_1^*)}{C_p}$

How do we do this design; x versus T. What is equilibrium curve? We know that it is k by k plus 1. So, we can calculate the value of k since, k value is given at 12.2 at 25. The heat of reaction is given. By using the Vantoff's equation, we can calculate the value of k at various temperatures and using that, we can plot this curve. Then, we also recognize that the locus of maximum reaction rates. Locus of maximum reaction rates is given by this x m by 1 minus of x m, equal to k E 1 by E 2. Using this relationship, we can plot maxima in reaction rate curve. This is x m; this is the x m curve; this is the x e curve. Then, if our feed temperature is given; feed temperature is given as 21. So, feed temperature is even as 21, but if you want to really, go to very high conversions, if we start with this as 21 and if you run a tubular reactor, which is our d t d x, we know that d t d x is given by C a 0 minus of delta H 1 star, divided by C p.

C p is given; C p is volumetric specific heat. So, we can we can now run a tubular reactor, corresponding to this slope; we can run a tubular reactor like this, and then we can stop somewhere here, but that does not take us to sufficiently, high conversion. Then, you run an interstage cooling. Then again, another tubular reactor, we run. Then, once again, we again, run. Then again, we do this. So, this is how we keep doing this, till we achieve the points of our interest. This is stage 1; this is stage 2 and stage 3. So, the exercise that we are looking at here is that what is the rationale for multi stage tubular reactor design? What is the rationale?

The rationale is that given a feed temperature and an adiabatic reactor at that feed temperature, if you run; at best, you can reach a conversion, which is much lower than what is desired in a process. If you want conversions from 95 percent and so on, that the process does not allow you to go such high conversions unless, you have multi stage designs. So, the design features that you must take into account is how much interstage cooling you would like to do between stages. You can cool up to here or cool up to here. Each decision implies a certain volume of the interstage cooling device and certain volume of the reaction. On other words, in multistage tubular reactor design, the volume of the reactor or size of the reactor, and size of the cooling device are both important.

Let us say for example, if you look at ammonia, is a high pressure process, or sulphur di oxide, which is a low pressure process, but it is gas. So, if this cooling is to be gas to gas cooling, would mean in very large heat exchange surface. You have a large heat exchange surface and therefore, a large investment here, and this is the reactor, depending upon the cost of the catalyst. You will find this tubular reactor would have a certain size. So, you have to take into account, the size of the reactor, as well as the size of the exchanger; both are the important from point of view of design. This is the point that you must bear in mind when we look at tubular reactor design. Both the size of the equipment, which is reaction equipment, and this is the heat exchange equipment; look at both to be able to decide what might be appropriate. So, this is the point I am trying get across to you. There are several good examples in the literature; shift conversion, steam reformation, ammonia synthesis, sulphur di oxide conversion and so on are fine examples of reactions where, the reaction reversible, exothermic and a catalytic and therefore, we need to do a multi stage design to be able to give you an optimum size of the equipment, at the same time, achieve very high levels of conversion.

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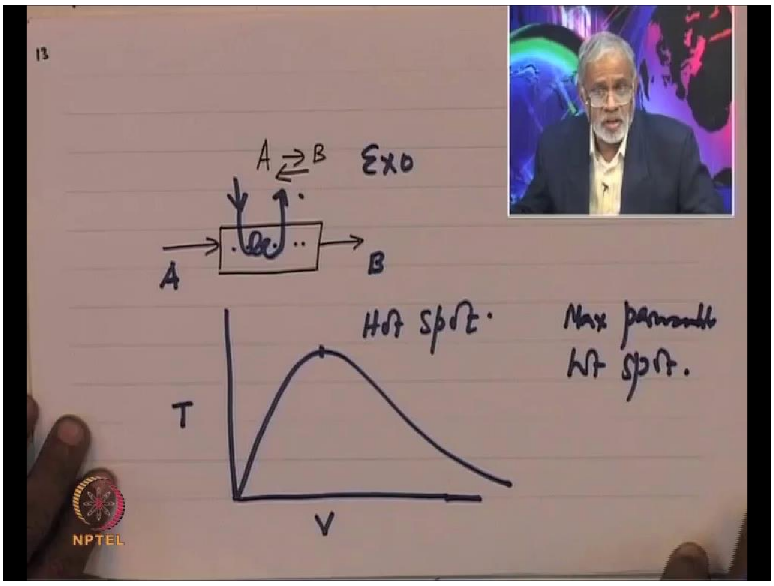

Having said this, there are some features that we must appreciate. Let me, sort of come back to this to illustrate what I want to say. What we want to recognize is that suppose, we have a tubular reactor. Let us say feed coming in, going out, because it is exothermic; A going to B as an example; B going to A. So, this is exothermic. What happens as a result, as it goes through, you will find; if you make a plot of temperature versus equipment, and if there is wall cooling; let us say there is some cooling here, coming in and going out; you will find temperature goes to maximum and comes down. On other words, there is a point called the hot spot.

What is the hot spot? Hot spot is the position where, the temperature of the catalyst becomes the highest. Generally, the reactor design should take into account, the maximum permissible hot spot temperature. Now, there are several reasons for this. One could be that the catalyst is not meant to be used at a temperature, higher than a certain specific temperature. Secondly, hot spot could be quiet high, and then there could be some bad effects on the material of construction of the equipments itself. In both the cases, we have to have a good idea of what the hot spot temperature is, and how we can regulate this.

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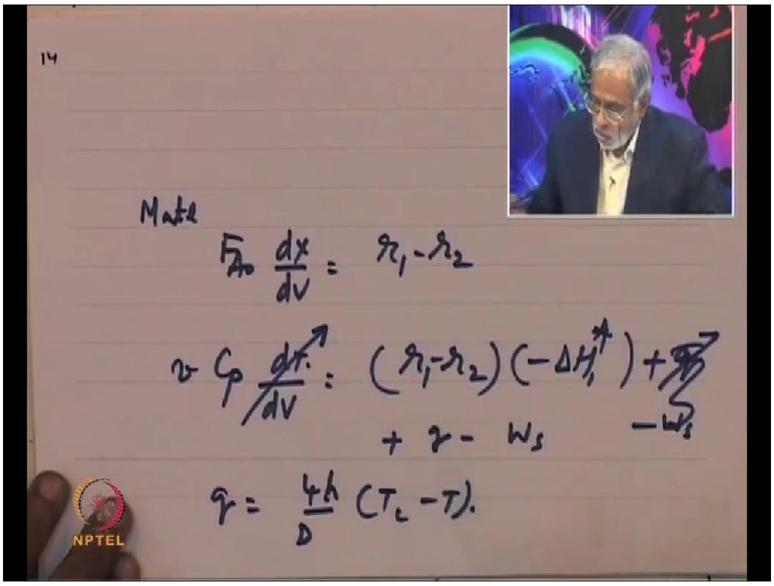

14

Mate

$$F_{A0} \frac{dx}{dV} = r_1 - r_2$$

$$v C_p \frac{dT}{dV} = (r_1 - r_2)(-\Delta H_1^*) + \cancel{q} \quad - W_s$$

$$+ q - W_s$$

$$q = \frac{4h}{D}(T_c - T).$$

Let us try and look at how to understand this by writing our equation, once again. So, let me write our tubular reactor equation, once again. We have our material balance, which is F a naught, times d x d v, equal to r 1 minus of r 2. Then, we have our energy balance, which is d t d v, equal to r 1 minus of r 2, minus of delta H 1 star, plus q minus w s, sorry, plus q minus of w s, and q, we shown; it can be replaced by this; T c minus of T where, H is the heat transfer coefficient; T c is the temperature of the heating medium. If it is a cooling medium, this T c minus T would be negative. So, it does not matter. If we look at this equation here, and I ask you what happens at the hot spot temperature; you will tell me that hot spot temperature, this term is 0. On other words, at the hot spot, the rate at heat generation, is balanced by the rate of heat removal.

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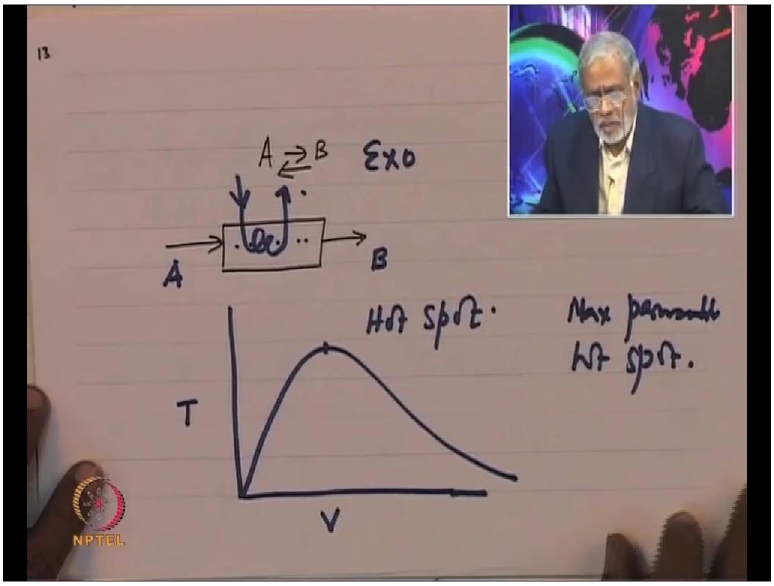

Consequently, you find that you will see a temperature profile like this. On other words, your tubular reactor temperature rises from T naught here, to various temperatures. Now, it might be useful to us, if instead of allowing a temperature variation in the equipment, if we can keep that temperature nearly constant, so that, we are able to ensure that hot spot problem, I mean, high, excessively, high temperatures are not encountered. At the same time, we are able to ensure that the reaction occurs at the temperature of our choosing; that is an advantage. The question that I would like to put across to you is that suppose, we want to run our process at a constant temperature; this is a condition that we want to impose on our catalyst for the reasons being that we want to be absolutely, sure that our catalyst is only exposed to temperature that we specify, and nothing more than that we are willing to accept.

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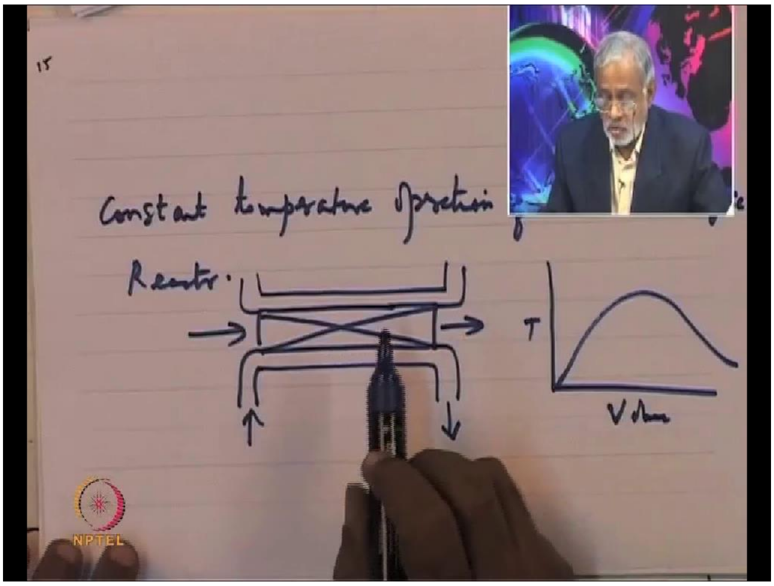

So, if there are situations like this, which you want to handle, how do we handle this? This is an example I want to illustrate. The example that I want to illustrate now, is constant temperature operation of a tubular reactor. How do you operate a tubular reactor at constant temperature? How can we do this and what does it tell us? Tubular reactor; catalytic, I say catalytic; that is important; catalytic tubular reactor, of course, what is in my mind is reaction such as steam reformation, shift conversion, ammonia synthesis, sulphur di oxide; great variety of reactions in the process industry where, you find that the temperature, I mean that the catalyst is essential for the success of the process. So, we have here, a reactor into which, there is a catalyst and feed comes in. There is what is called as a jacket; this is a jacket, and through which, a cooling fluid goes in and comes out.

Now, because of the fact that there is a wall cooling, we are seeing this kind of temperature as I pointed out to you; T versus volume, and we do not want this. How do we design and operate the process, so that, this variation in temperature is not an issue in our process? This is what we want to do; how do we do this? To be able to do this, just want to set up our equations, once again, and recall our interest in.

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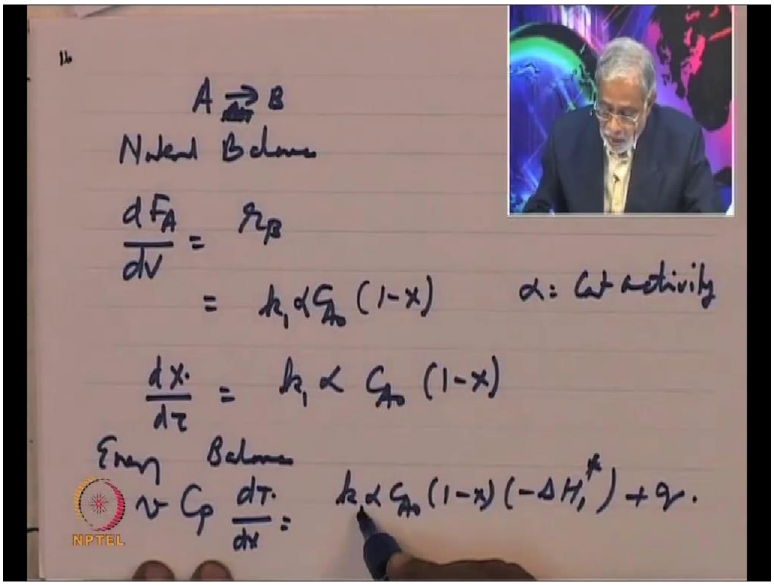

$A \xrightarrow[\alpha]{} B$

Material Balance

$$\frac{dF_A}{dV} = r_B = k_1 \alpha C_{A0}(1-x) \qquad \alpha : \text{Cat activity}$$

$$\frac{dx}{d\tau} = k_1 \alpha C_{A0}(1-x)$$

Energy Balance

$$v C_p \frac{dT}{dV} = k_1 \alpha C_{A0}(1-x)(-\Delta H_1^{*}) + q.$$

So, we are going to have B as our reaction. We have this, our material balance, given by this, all right, and then this, I call this r b as some k 1 C a 0, 1 minus of x. I will take for the moment, irreversible reaction; we can relax it a little later. Now, let us say add to the catalyst alpha. So, this is our reaction, is taking place. I will put it in the form of d x d tau equal to k 1 alpha C a 0 times of 1 minus of x where, alpha is catalyst activity, all right. So, this is the material balance. Now, how does our energy balance look like? Our energy balance looks like this; v C p, d t d v equal to k alpha C a 0, 1 minus of x, minus of delta H 1 star, plus q; I just mean, in our energy balance, we have written it earlier. We have just replaced the reaction rate with the rate function here, all right. So, this is k 1. Now, what we said? What we said; let me say it once again.

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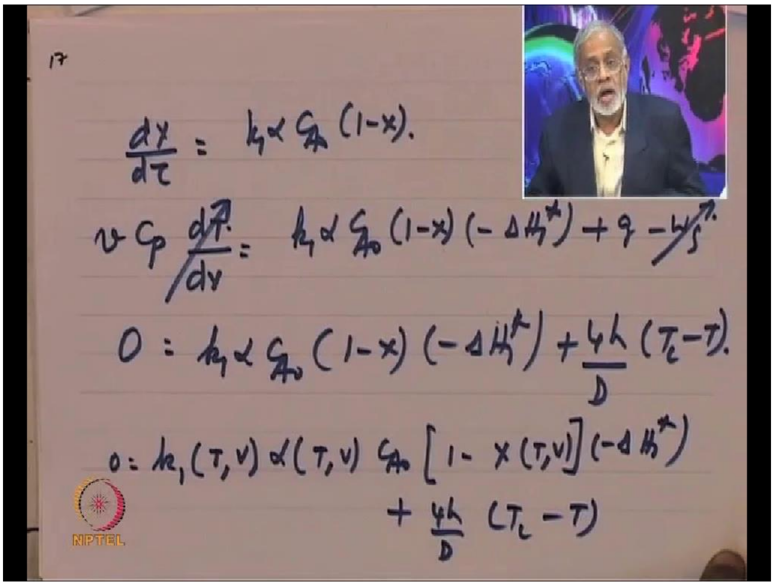

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$$\frac{dx}{d\tau} = k_1 \alpha C_{A0} (1-x).$$

$$v C_p \frac{dT}{dv} = k_1 \alpha C_{A0} (1-x)(-\Delta H_1^*) + q \cancel{- W_s}$$

$$0 = k_1 \alpha C_{A0} (1-x)(-\Delta H_1^*) + \frac{4h}{D}(T_c - T).$$

$$0 = k_1(T,v)\, \alpha(T,v)\, C_{A0} [1 - x(T,v)](-\Delta H_1^*) + \frac{4h}{D}(T_c - T)$$

Our energy balance; I just want to write it once again, to emphasize d t d v equal to k 1 alpha C a 0 times of 1 minus of x, minus of delta H 1 star, plus q. Of course, minus w s, we are not going to derive, work out this, and then d x d tau equal to k 1 alpha C a 0 times 1 minus of x. We want to run our process at constant temperature. On other words, we do not want any variations of temperature in this equipment. We do not want that, which means what; which means that we want this to be 0, correct. How do we get that left hand side to be 0, which means, this terms k 1 alpha C a 0, 1 minus of x and this q; let me write this in this form; k 1 alpha 0, equal to 1 minus of x times minus of delta H 1 star, plus 4 h by d; this we have done before; I am just writing it once again, this. So, this is our T c, is going in, coming out; this is T 0, and then temperature coming out is T. So, we do not want any variations between T 0 and T, and T 0 is chosen as per our understanding; may be 200, 250, 300; whatever is the temperature at which, you want the equipment to perform.

So, T 0; whatever is the T 0 temperature at which, it emerges and this temperature, there is no change in temperature here. Only reaction occurs, which means what? This temperature, this k 1, this temperature at which, the reaction occurs; this is the rate of heat released and the rate of heat, being picked up by the cooling device. So, this rate of heat generation must be equal to rate of heat removal, and this must be. So, at every point, the point we are saying is that k 1; 0 equal to k 1; temperature at any position; alpha at any position; C a 0, 1 minus of x at any position; minus of delta H 1 star, plus 4 h by d, T c minus of T; this must hold at every point in the equipment. This relationship must hold at every point in the equipment. How do we do this?

This is the point that I am putting across to you, because if we can do this, the operation of tubular reactors that we will face in process industry; constant temperature would have great advantage from the point of view of looking after the activity of the catalyst and even, running the process, the kind of benefits you will be getting at constant temperature, is a great advantage. So, we want to see by looking at the equation, what is that you and I can do to ensure that this equality is maintained at every point in the reaction equipment. Let us see how to do this. So, what have we said?

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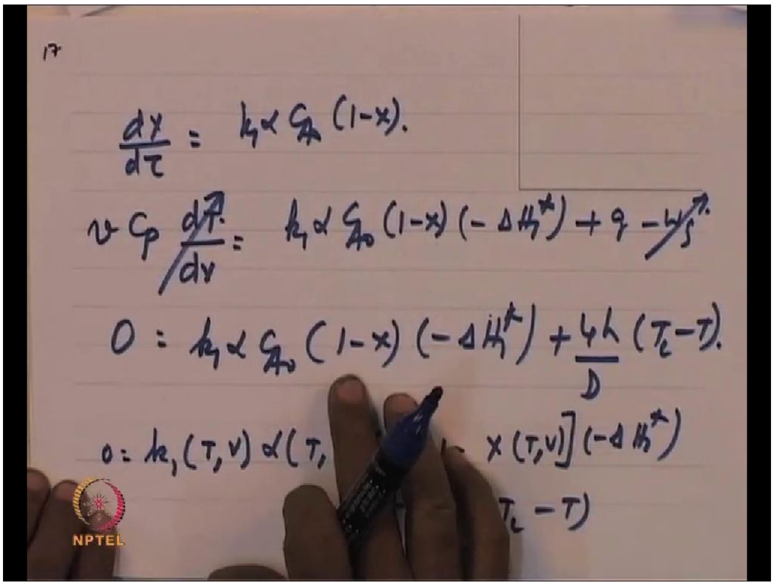

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$$\frac{dx}{d\tau} = k_1 \alpha C_{A0} (1-x).$$

$$v c_p \frac{dT}{dv} = k_1 \alpha C_{A0} (1-x)(-\Delta H^*) + q \cancel{- \frac{4h}{D}}$$

$$0 = k_1 \alpha C_{A0} (1-x)(-\Delta H^*) + \frac{4h}{D}(T_c - T).$$

$$0 = k_1(T, v)\, \alpha(T, \quad x(T, v)](-\Delta H^*)$$

$$T_c - T)$$

We said we want this left hand side to be 0. What it means; which means, this is equal to q; that means q must be equal to this term.

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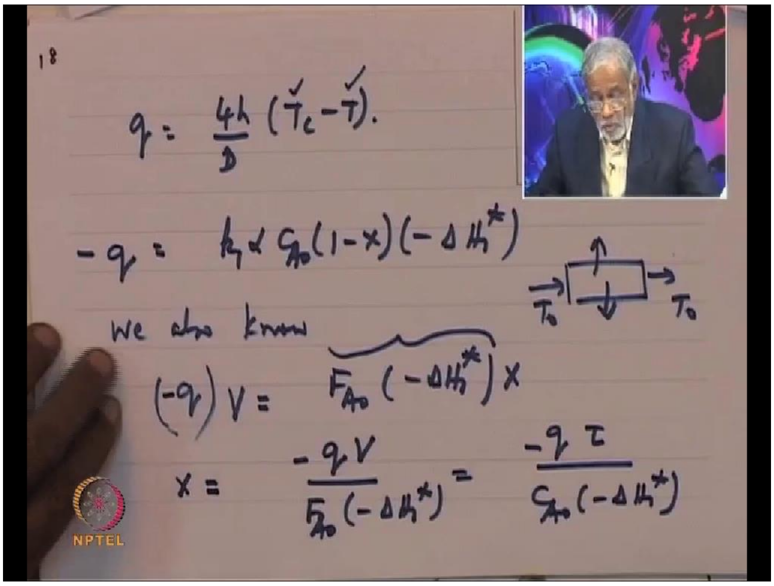

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$$q = \frac{4h}{D}(\overset{\checkmark}{T_c} - \overset{\checkmark}{T}).$$

$$-q = k_1 \alpha C_{A0}(1-x)(-\Delta H_1^*)$$

$$\xrightarrow{T_0} \boxed{\uparrow \ \downarrow} \xrightarrow{T_0}$$

We also know

$$(-q)\,V = \overbrace{F_{A0}(-\Delta H_1^*)}\,x$$

$$x = \frac{-qV}{F_{A0}(-\Delta H_1^*)} = \frac{-q\tau}{C_{A0}(-\Delta H_1^*)}$$

Let me write, which means, q equal to k 1 alpha C a 0, 1 minus of x times minus delta H 1 star, minus q equal to, because q by definition, is 4 h by d, T c minus of T. So, minus q means T is greater than T c; that is all it means. What is q? We also know that q, which is heat removal per unit volume, multiplied with the volume of equipment, must be equal to F a 0 minus delta H 1 star times x; do we agree with this? What we are saying is that the total amount of heat released; that heat is taken up by the cooling fluid. The reason is where will this heat go; anywhere. Whatever the heat that is released by process; where can it go, because it is not increasing the temperature of the fluids, because the fluids are at the temperature at which, it is entering.

What we are saying is that the reactor whatever, is the temperature at which, it is entering; it is leaving at that temperature only. Therefore, the only way this heat can escape is into the cooling fluid. So, this is the statement of that energy balance; q times, I put a minus sign here; q times v equal to F a 0 times delta H 1 star times x. Let us say understand whether, this is positive, minus delta H 1 star is positive for an exothermic reaction. So, right hand side is positive. What is left hand side? For x, left hand side T is greater than T c for the system where, there is cooling; therefore, this is also positive. So, it is quiet consistent. So, what we get out of this is x equal to q v by F a 0 minus of delta H 1 star with minus or it is also equal to q tau, divided by C a 0 times minus delta H 1 star; is that clear, what we are saying?

We know from our understanding of the physics of the process that whatever, the heat is generated by the reaction, is taken up by the cooling fluid. I put a negative sign here, because it is first law convention; q is formulated as heat; put into the system. Here, heat is removed from the system. That is why I put a negative sign. So, it says that the extent of the reaction, as by this definition, is given by q v by F a 0 delta H 1star or in this form.

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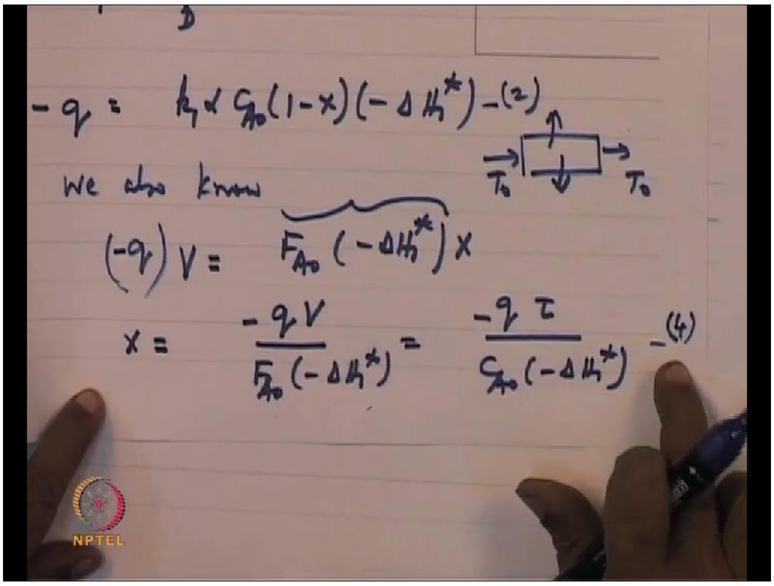

$$-q = k_1 \alpha C_{A0}(1-x)(-\Delta H_1^*) \quad -(2)$$

We also know

$$(-q)V = \overbrace{F_{A0}(-\Delta H_1^*)}\, x$$

$$x = \frac{-qV}{F_{A0}(-\Delta H_1^*)} = \frac{-q\tau}{C_{A0}(-\Delta H_1^*)} \quad -(4)$$

Now, we notice here, we are going to substitute for x from this equation, into this equation. So, I will call this equation as, I will put a number just to; I put this as equation 2, and therefore, this as equation 4. This is what I have in my note books,, so you will bare with me. So, I want to substitute for x from equation 4 into equation 2; that is all I am going to do now.

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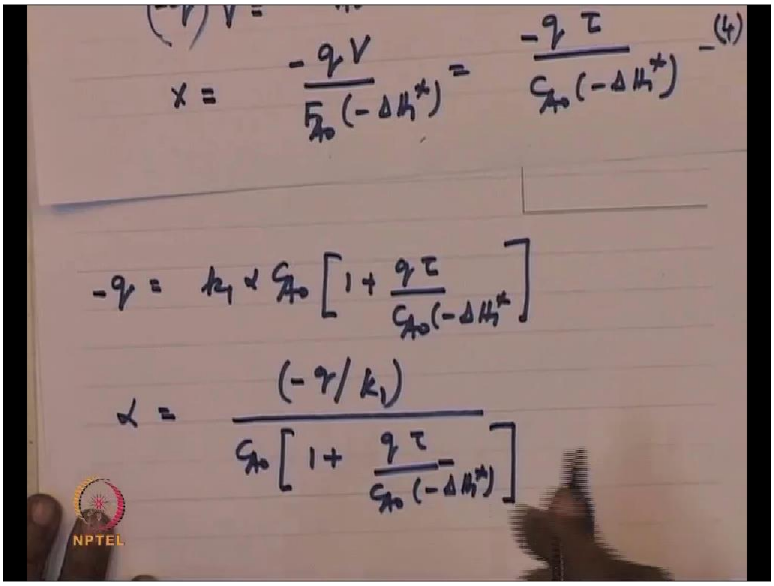

$$x = \frac{-qV}{C_{A0}(-\Delta H_1^*)} = \frac{-q\tau}{C_{A0}(-\Delta H_1^*)} \quad -(4)$$

$$-q = k_1 \alpha C_{A0}\left[1 + \frac{q\tau}{C_{A0}(-\Delta H_1^*)}\right]$$

$$\alpha = \frac{(-q/k_1)}{C_{A0}\left[1 + \frac{q\tau}{C_{A0}(-\Delta H_1^*)}\right]}$$

When you do this, you get q equal to k 1 alpha C a 0, 1 minus x is what; q tau, divided by C a 0 times minus of delta H 1 star; is this clear? What are we doing? This is minus q. I am substituting x from 4 into 2. So, minus q equal to k 1 alpha; I have just written exactly, what I have written and minus of x; since, x has got a minus sign, I put a plus, all right. So, this equation gives us alpha equal to minus of q by k 1, divided by alpha equal to q by k 1, divided by C a 0, within bracket, 1 plus q tau, divided by C a 0 times minus of delta H 1 star. Let me just make small simplification, just to make it look a little nice. So, I will just simplify it slightly.

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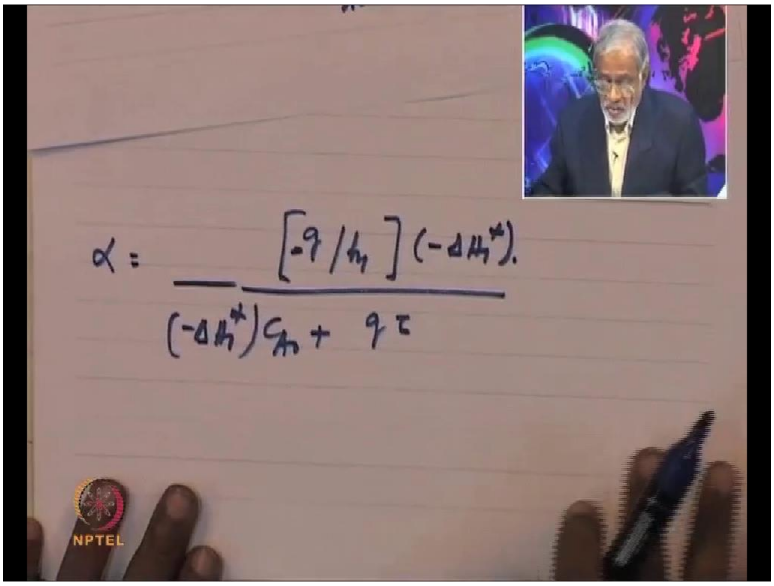

$$\alpha = \frac{[-q/k_1](-\Delta H_1^*)}{(-\Delta H_1^*)C_{A0} + q\tau}$$

So, alpha equal to q by k 1 with a minus sign, divided by; I take C a 0 common. So, it becomes C a 0 plus q tau, divided by q tau delta H 1 star, with a minus sign; have you got it right? Then, there will be a minus delta H 1 star in numerator; is that correct? Please tell me, have you got it right? Taking common C a 0, cancels off; minus delta H 1 star goes up; it is fine. So, what are we saying now? What we are saying is that what is alpha? Alpha is catalyst activity. Now, what can we do, which means that we can change the activity of the catalyst by putting active catalyst along with some amount of inert.

On other words, by mixing the catalyst with some inert, we can actually, change the activity of catalyst that we are going to put inside the reaction equipment. Now, what this equation saying is that if you want to maintain the temperature of the reactor, constant across the reactor, if this temperature has to be constant everywhere, then the catalyst activity; that means, the amount of catalyst we will put here, put here and put here; this should be changed and that program of change is going to be described by this equation; that means, you must change the amount of catalyst that you are going to put into unit volume of the reaction equipment here, and here, and here and so on; it should be described by this equation. On other words, you have to exercise lot of care in filling a reactor with catalyst, and if you fill the reactor with catalyst as per this equation, then your reactor will perform at the temperature that you have chosen. Therefore, you have gotten rid of one the most difficult problems of trying to operate a chemical reactor, because this chemical reactor will run exactly, at the temperature at which, you have designed. Now, let us just put it in another slightly different form, so that, we can appreciate the usefulness of the equation.

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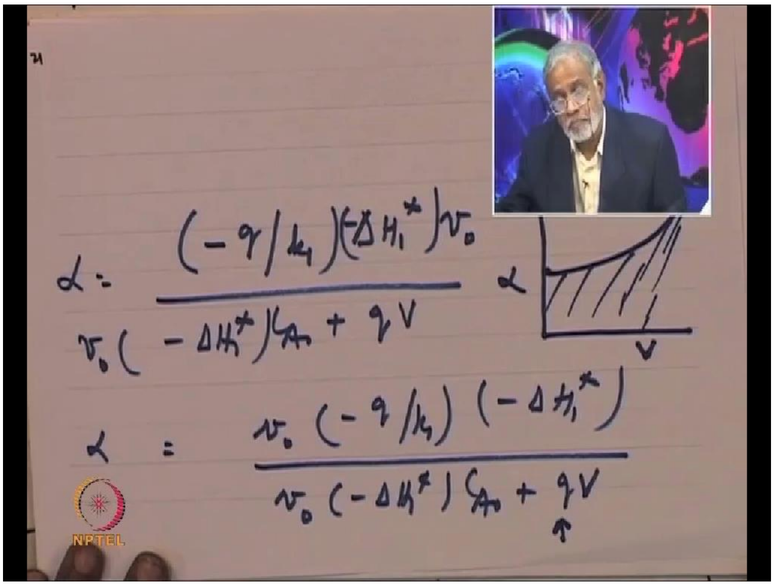

$$\alpha = \frac{(-q/k_1)(-\Delta H_1^*)v_0}{v_0(-\Delta H_1^*)C_{a0} + qV}$$

$$\alpha = \frac{v_0(-q/k_1)(-\Delta H_1^*)}{v_0(-\Delta H_1^*)C_{a0} + qV}$$

Alpha equal to minus of q by k 1 minus of delta H 1 star with the minus sign, divided by minus of delta H 1 star times C a 0, plus q, we can tau as q divided by v 0. So, I can put v 0 here; I can put v 0 here. On other words, what we are saying is that v 0 times minus of q by k 1, minus of delta H 1 star, divided by v 0, minus of delta H 1 star C a 0 plus q v, equal to alpha. So, what we are saying now, is that if you make a plot of alpha versus v, as v increases, alpha decreases. Please note that q is negative. Therefore, as v increases, the denominator keeps on decreasing and therefore, you will find that if we start here, and then therefore, alpha keeps on increasing; therefore, we are actually, putting a higher and higher amount of catalyst at later positions in the equipment, because of this program of catalyst laying inside the reactor, you are able to maintain the constant temperature.

So, it is this profile of catalyst loading in reaction equipment; that ensures that you will get uniform temperature throughout the equipment. Let us ask one more question; all right, we have done our design for at a given temperature T equal to 220, all right, C a 0 equal to some value, or v 0 equal to some value. Now in a process, C a 0 might change; v 0 might change. So, many things may happen in your process. How do we manage to run a process at constant temperature, despite variations in all these kinds of processes? Now, we can understand this and we can also, address these things, quiet easily now by looking at these equations we have written now. Let us say, let us take an example to illustrate what I am saying.

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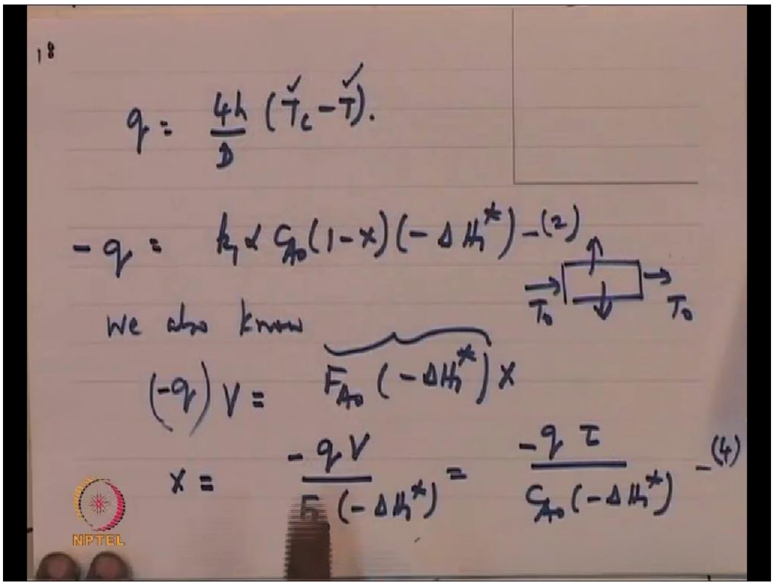

$$q = \frac{4h}{D}(\overset{\checkmark}{T_c} - \overset{\checkmark}{T}).$$

$$-q = k_1 \alpha C_{A0}(1-x)(-\Delta H^*) \text{ -(2)}$$

We also know

$$(-q)V = \overbrace{F_{A0}(-\Delta H^*)}x$$

$$x = \frac{-qV}{F(-\Delta H^*)} = \frac{-q\tau}{C_{A0}(-\Delta H^*)} \text{ -(4)}$$

What we are saying now? We are saying that C a 0 has changed; C a 0 has been increased or decreased, let us say. So, C a 0 has changed; that means, if you want to maintain this heat release, this must be equal to q. How do we ensure this equality? This q is given by this quantity; 4 h by d T c. On other words, we can adjust T c to get our temperature T or alternatively, if you do not adjust T, your temperature will automatically, reset. Instead of operating at 220, you may operate at 215 or 225. In both cases, you will still be operating at a constant temperature. That is the point I am trying to put across to you; that this design gives you an opportunity to operate a process at a constant temperature, but you do not want to run at a temperature, which is more than the temperature you prefer.

On other words, if your design is only 220, and you do not want it to be more than 220, clearly, you do not want a higher value, a different value of C a 0. If it is going to give a higher temperature, you do not want it, in which case, you will have to reset your T c, so that, it takes place. On other words, here is an instance of a design, which gives you a lot of control over managing the quality of the catalyst, so that, the catalyst life is preserved; catalyst performance remains as you have designed, and your process control becomes much easier than what you would anticipate. So, just to cut this long story short, what I am trying to say in tubular reactor design is that this approach of trying to maintain constant, might be of great value, particularly, with expensive catalyst that we often encounter in the process industry.

Thank you.