Chemical Reaction Engineering 1 (Homogeneous Reactors)

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Lecture No 42

Non-Isothermal Reactors (Graphical Design) Contd.

Okay I think we will start now our non-isothermal reactor design, graphical design only one part is left I hope you have understood okay or did you enjoy doing that? There is so beautiful I said very simple very simple way of doing things but it is not easy for you to do on your own because I think I have drawn the lines just like that but you have to calculate those lines and then you have to draw and this activation energy and also you know this Delta H r will give you help particularly the units because you have activation energy coming there in K values and K by mistake if you are not able to even put proper dimensions you will never get those lines.

So that is why you have to be very careful and drawing those lines anyway today I will give you also one exercise so that you know you will practice out to draw those lines and we will draw I will give the exercise only for irreversible reaction because that is slightly complicated no reversible reaction, reversible reaction which is complicated and then I think you know when you do complicated things uncomplicated things are very simple so that is the reason okay good. So the last part is left in graphical design is, is there an optimal design or this you know using graph okay (())(1:34) also we have the same question is there an optimal design okay what do you mean by optimal design?

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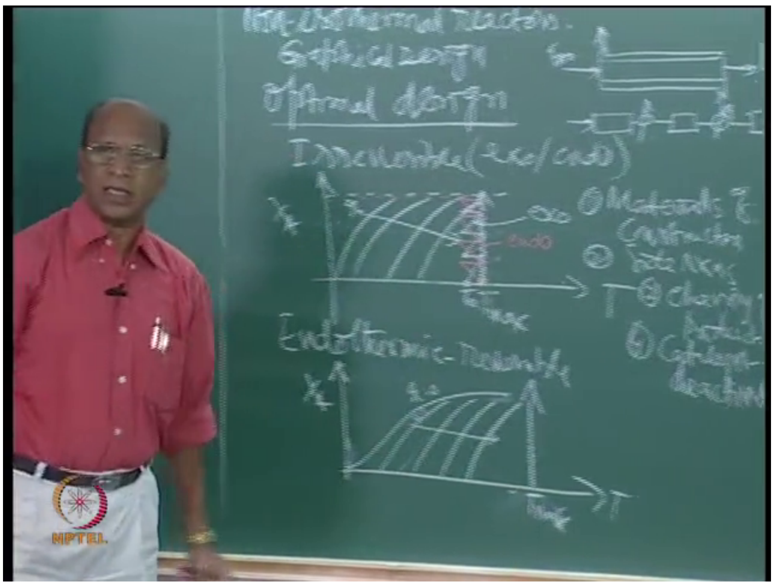

What do you mean by optimal design? Yes okay that minimum volume that is possible for a given conversion or maximum conversion that is possible for a given volume okay and if it is multiple reaction what is the optimal problem there? This is straightforward single reaction, when I have multiple reactions what…?

Student: (())(2:15)

Professor: Yes it is not the volume there it is the yield there okay yield or selectivity both are same the way you define okay yes, so there the question is you do not worry about whether the reactor is smaller or larger there okay, so that is why you always question there at okay how much yield I can get because that particular product may be having very high cost, so that is why even if you forget about the total volume of the reactor by producing more and more of that particular compound in terms of yield okay then you will have to then you may your plant may get a lot of profit.

So that is the reason why that question is different right? But still you have to also find out what is the volume of the reactor for that equivalent yield, that equivalent yield given by what conversion and use that conversion to again calculate the volume using the same procedures what we have done? So here now optimal design what we discussed is that if it is irreversible exo or endo what is the optimisation? So I have here X A versus T graph, so now for irreversible you know what kind of graphs is we get, what kind of graph we get? Like this you get good yes, now how do I use this information for getting minimum volume for the given conversion, what is the strategy? Have already some information in your brain okay, so when do you get the minimum volume?

Student: (())(4:00) is maximum.

Professor: Excellent Abdul okay so when the rate is maximum, so when do you get the rate maximum here?

Student: At high temperatures.

Professor: At the highest temperature that is possible because as the temperature is increasing here the rate is increasing this is r okay so that means I can go on drawing till the end you know the line and then draw the temperature but is there a limit? Highest temperature you know the first question what I asked was what do you mean by the minimum volume here when do you get? So if you remember the design expression and he remembered and you told that when you get the highest rate and you will get the minimum volume and that highest rate be given by here highest temperature because the temperature is involved here okay. So and what is that highest temperature that is possible?

Another question here, so the highest temperature means is it…you told that highest rate, do you get this rate at 1 temperature or at various temperatures? In this case we are talking irreversible reactions, so that means what for irreversible exothermic or endothermic what should be now the strategy and I am very happy that you are able to answer all correctly exothermic or endothermic, what is the strategy I mean though the temperature you said corresponding to a particular temperature you will get the highest rate okay. So now what is the temperature and what kind of temperature scheme I should have in the reactor? Is it 1 temperature, so that means what you call that, if throughout the reactor you have 1 temperature?

Student: (())(5:49)

Professor: Excellent (())(5:50) you should have isothermal temperature highest that is possible this is T max, how do I decide now that T max?

Student: (())(6:06)

Professor: Yes (())(6:07) will come at the end and before that (())(6:09). Someone was telling which conversion?

Student: (())(6:16)

Professor: How do I choose that T max, you have ideas already I told you also just think.

Student: (())(6:28)

Professor: Conversion is fixed for a given conversion we are talking.

Student: (())(6:36)

Professor: How do I choose that T max?

Student: Rate of increase will be different.

Professor: Rate will be higher that is why we (())(6:44) that T max.

Student: After certain temperature…

Professor: (())(6:51) you do not have a choice that is why it should be kinetic.

Student: After certain temperature the rate will not be that much increasing.

Professor: No as temperature increases again you are coming back to the other wrong answer because you already decided that as temperature increases the rate will be increasing continuously again you cannot say the rate decreases after sometime.

Student: I am not saying the rate decreases…

Student: (())(7:17)

Professor: Yes how do I decide that operating temperature? Abhishek already have given the answer. Yes highest temperature…

Student: Reactor should withstand.

Professor: Reactor should withstand that means what is the factor that comes (())(7:33) of construction that is one other one…

Student: Products are (())(7:37) should be stable.

Professor: Yes at high temperature they may be side reactions which you do not like okay even though there is a multiple reaction sorry single reaction, so at one point of time you do not know there may be separate another reaction coming is not possible you should not allow that then any other thing?

Student: (())(7:56) which the reactor can withstand beyond that it will not.

Professor: That is what he said I think that the (())(8:03) of construction beyond which the material should mix in that kind of temperature okay and also another thing. The product formation and also (())(8:13) products you know some of the products may get burned and everything you get only carbon okay at the end, so that is why we do not want carbon including reactor if you go behind certain values okay, so that is why T max is decided by now yes materials of construction yes that is one and also side reactions and number 3 is charring of products yes this is true even for heterogeneous reactions the similar things what the same rules can be extended but if it is catalytic reaction what is the 4^{th} one? catalyst should withstand I think most of the time catalyst will control (())(9:14) of constructions and all that there is no problem okay catalyst will control because catalyst should not be thermally deactivated.

So catalyst deactivation okay, so all these things will come for this irreversible, so it is very easy now for us to remember that okay graphical design will tell me that I have to go for highest temperature because the rates are increasing as I increase the temperature and now the scheme should be isothermal that means throughout the reactor I should have the same temperature, now the question is how do I maintain that that particular temperature because throughout I should maintain the same highest possible temperature, how do I do that?

If it is exothermic reaction or endothermic reaction okay yes I think before answering those questions is take this yes I think you know the optimal design, optimal design means you know minimum value or maximum conversion depending on what is the parameter which you are going to use. Optimal design depends on the optimum temperature progression which minimises V by F A not for a given conversion, the optimum may be an isothermal or it may be a change in temperature in time for batch reactor, along the length in PFR And stage to stage or a series of MFR's.

Next para you can write it is important to know what this progression is because it is the ideal which we try to approach with a real system, it also allows us to estimate how far any real system departs from the ideal okay good. Next para please write the condition for optimum temperature progression in a given type of reactor is as follows whatever the composition always have the system where the rate is maximum very simple rule, so I think inverted comas if you started you just close it okay, so that means you know I mean whatever may be the composition look at the temperature where you get the maximum…for that temperature what is the maximum rate?

So when you are putting together all these rates for example in a PFR okay all the maximum rates then the reactor volume will be minimum because in the denominator average of all that rates only will be there if you say PFR, if it is batch same thing again batch and PFR simply replaced by you know space is replaced by time okay and if it is MFR we have only one rate and also you know one temperature and 1 conversion correspondingly, so we know how to find out that maximum rate because we know what is the corresponding temperature and conversion and also corresponding rate, so whether that is highest not okay. So now next one what you just write is after that, the locus of maximum rates is found by examining XA versus T graph okay so that is what we have done here. This is X A versus T graph right and now we thought that rate is increasing as we increase the temperature.

So you can go and go further whatever temperature you want but we have restrictions these things, so you have to choose the highest any one of the 1 okay the lowest of these things because even if the catalyst is getting deactivated and materials of construction it may withstand maybe 2000 degrees Celsius but catalyst is getting (())(12:59) after 600 you cannot go there okay so that is lowest of this will decide which one will be the r side reaction may be taking place at point (())(13:07) maybe right so that is one what we have to choose and within that now you have to try to get this what is the minimum volume for a given conversion or vice versa the (())(13:18) it prove okay good so now for irreversible reactions please take this for irreversible reactions that we have already discussed for irreversible reactions the rate always increases with temperature at any composition.

So the highest rate occurs at the highest allowable temperature this temperature is set by materials of constructions, side reactions, catalyst deactivation et cetera good excellent, so now the second one this is the first one irreversible we have now endothermic a reversible reaction, endothermic reversible okay yes before going to that endothermic reversible you see here yes I think the practical thing I wanted to ask you how do you maintain this isothermality if I have a plug flow? It is easy to maintain in mixed flow, right yes. So whether I have to heat or cool to get that temperature if it is highly exothermic but you know sometimes if the rate is lower beyond certain temperature I have to remove some heat and then maintain that temperature so that I will get the highest rate that is no problem but for plug flow and also batch reactor what do you do? Just I want you thinking that is all I think you know how do you imagine these?

See by putting just blindly one heat exchanger like this, this is plug flow, so maybe this is you can put it in the other way also no problem yes, so this way this is of course F A not entering F A coming out, so now how do I maintain the isothermal that means every cross-section I should have the same temperature then only you will get the real optimum that is the reason why I told this is the ideal situation that is the most ideal case and now how do you maintain that kind of temperature? I think theoretically we also told you there is no isothermal condition anywhere in plug flow unless you put infinite number of heat exchange that means very small cross-section I have to take and then I have to put an heat exchanger to effectively control the temperature in that cross-section okay and cross-section you can put infinity along the length so that is the reason why you do not have that kind of ideality.

So that is why you have to now…in reality you will just go slightly away from the ideality that is what I think all of us to okay. You are all young when we are all very young you know what we imagine is that the most beautiful girl on this planet should be my wife okay true boys, girls also same thing the most handsome guy on this planet should be…but the reality is different okay the reality is totally different okay because I think how many most beautiful girls you can find in this planet, so whoever you get she is most beautiful for you, so that is the actual adjustment with the ideal world, correct? So that is what is the ideality you know deviation from ideality that is what we know what we can do here, so one way of doing that is if I have exothermic reaction how do I maintain but this is very nice very beautiful if I have exothermic reaction how do I maintain isothermality?

So that means infinite number of the heat exchange I cannot put, so I have to go some finite number may be 10 maybe 5 how do I do that, how we will do is you cannot cross this was the moment you cross one of these things will control and you can spoil the entire reaction so you start as much as possible yes if you are using adiabatic reactor that is one of the simplest one instead of putting jacket around you put adiabatic reactor no jacket or no heat removal system around the reactor but you do all that heat transfer after the reaction that section is over.

So that means you use now multistage small portion heat exchangers, small portion heat exchanger how much is this small portion that depends on again you retransfer and coolant and all that so you start that means adiabatic system you are using reactor is adiabatic but in between you have heat exchanger, so if it is exothermic reaction I will start even this is also a parameter even T not also which one is the correct T not also is a parameter through optimisation one can find out that, so now because it is adiabatic exothermic how it moves? It moves like this but then I have to… that means I have to see my calculation that a temperature increases along the length of the reactor conversion and then it goes to maximum this value correct beyond that I cannot go then what I have to do? Heat exchanger I have to use, when I am using heat exchanger there is no reaction right so then what kind of line I can draw here?

Student: (())(18:55)

Professor: How it can come down?

Student: (())(18:58)

Professor: How it can come down because I think see conversion see I told you there is no reaction, so what should be conversion?

Student: Same.

Professor: It is same, so now it has reached this conversion, so that means in how far you have to go again it is an optimisation problem and then not to say that you found that and again you go here and again go here, so what is the type of reactor now what we have here? Section yes this is heat exchanger again another section heat exchanger another section like that you know how many you need, so this is reactor and it need not be same length sometimes you know it will be decreasing in progression, sometimes it will be increasing in progression probably if it is endothermic reaction, now endothermic reaction what you do?

Student: (())(20:02)

Professor: It is not (())(20:05) how it is isothermal? Because I cannot get that kind of isothermal okay yes I think this question is good (())(20:14) so good so to really become isothermal I have to move only on that that is why we are telling we have in finite number of times right here I have put but that means I have to start here, go here, start here, go here, start here, go here so that means in finite number I want, what Rajesh Shree?

Student: (())(20:40)

Professor: Yes I know the assumption is that there is no the moment it comes out of the reactor okay you have to assume that there is no reaction which is not correct particularly for homogeneous reactions okay that is correct for catalytic reaction because there is no catalyst no reaction that is why you know I think that sulphur dioxide to sulphur trioxide also it is used I will tell you that one later, so like this but now if I have endothermic action and what do I do? I start with this point that is highest possible right but now temperature decreases though this goes this side, so this one so this goes this side right that means temperature falls and also conversion of course is increasing then you have to see where you have to again heat now because you have to be on this line as much as possible then again so like this (())(21:51) your conversion that is the length that is the final conversion okay.

So like that you have to do see how thrilling it is if you really do because you are not doing you do not really enjoy it okay I do not know whether it is fortunately not doing or doing unfortunately not doing because this is what is true chemical engineering I say there are so many things there are so many wonderful things that are happening and people have been using this already but only thing is I think even at this point in time you will get excited provided you have interest in designing this chemical engineering equipment, so that is how what we do for exothermic or endothermic and red one I will write is Endo and this white one we will write it as exo, so that is how and as I told you infinite means you will practically lie on this line that is isothermal throughout (())(22:47).

So inside you have…definitely there is some small variation of temperature but if I take this kind of length from here to here they may be 15-20 degree variation are fired a very close here and then try to do there may be only 1 degree variation, so practically almost you may get isothermal conditions when you go to the overall name, so that is how for exothermic endothermic it is done okay good.

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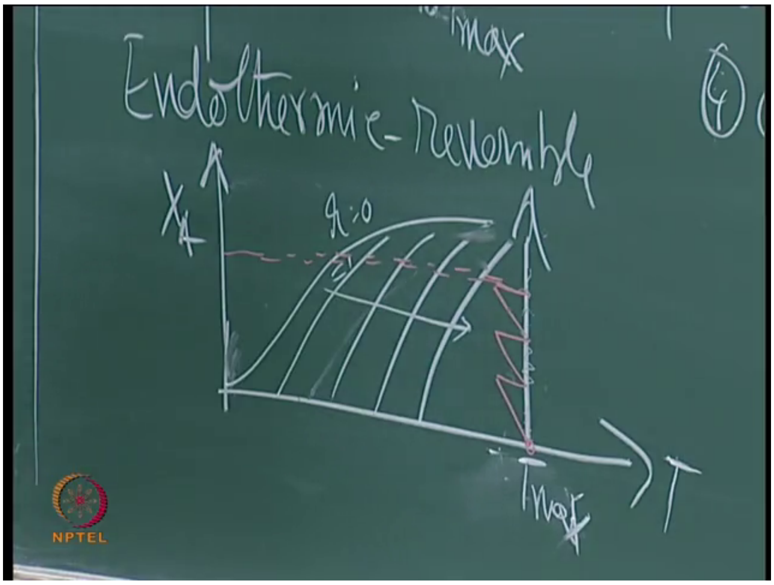

Now reversible this is endothermic reaction reversible, what is the kind of X versus T you get here this is X A versus T okay then we have r equal to 0 something like this correct this is r equal to 0 that is equilibrium (())(23:34) 0 equilibrium conversion and corresponding temperatures good. So now if I, this will be like this again how the rate is… it cannot touch there yes so rate is increasing like this only r equal to 0 may be r equal to 1 here, so like that it increases. Now what is the condition for here optimal progression that means even here we can clearly see that as temperature is increasing rate is increasing, so limit is again T max yes straight T max this is T max.

So now of course here again if you want to be exactly on the line so there will be infinite number of heat exchangers along the line okay but this is endothermic it is very easy now to draw because we have already done here, so we start with the highest rate I mean highest yes temperature corresponding to that highest rate, right. So then I will draw like this, like this, like this if I am going for yes may be the conversion required is this much yes then I need 1, 2, 3 reactors and 3 heat exchanger okay good. So this is actually not that thrilling when compared to your reversible exothermic.

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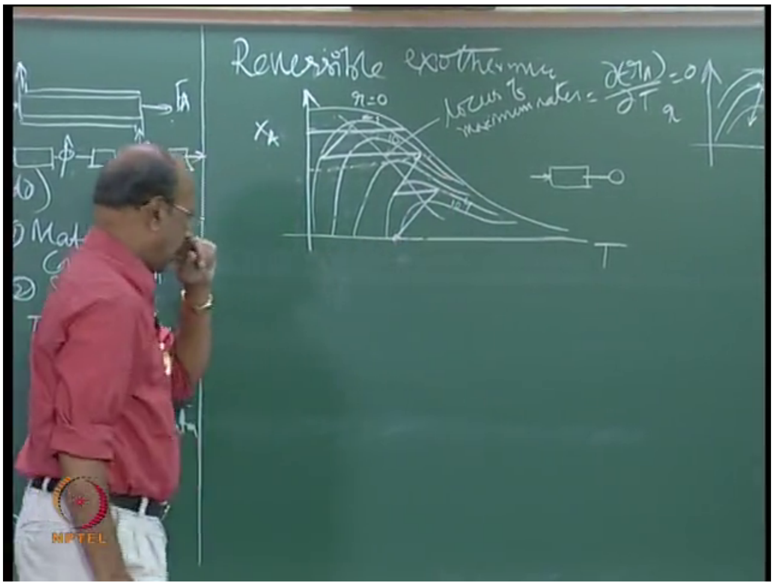

Reversible exothermic you know the plots here X A versus T, here yes this is r equal to 0 and we know that as temperature is increasing you will have conversion falling, equilibrium conversion itself is falling and you cannot cross equilibrium conversion, so that is why conversion falls in a reactor where temperature is increasing and the rates if you calculate and then plot you may get something like this yes rates are increasing like this. This is 1 okay 10, 100, 1000, 10000 okay this is 10 to the power 4 okay in between you have the lines yes. So here this is exciting the reason is that it is not a blindly as temperature is increasing you have you know the rate also increasing rate, rate is increasing there is no problem at all as temperature you see as when compared to this rate this is definitely more right,

So but the achievable conversion decreases that is thermodynamic limitation that is why this is one problem where kinetics and thermodynamics both play a role okay there also it is playing but this is quite dramatic in the sense that you cannot cross thermodynamics here, right. So that is why what we do here is that we start at high temperatures okay we started definitely at high temperatures yes okay before that when we started at high-temperature we will come later but what are the maximum rate curves here maximum rate line will be connecting these (())(27:31) this is locus of maximum rates.

So some of you may not be easily you know may not be understanding this one that easily why they are called actually this is a different rate, this is different rate, this is different rate and I am telling that that is the maximum rates okay. If you plot X versus T it is not quite obvious but X versus T is the best way for design right, so but actually if I plot rate versus temperature and this line is nothing but doh r by doh T equal to 0 that the maximum locus line okay and that is what. You can actually derive you can actually differentiate that and try to find out the temperature and corresponding rates okay or corresponding conversions also okay good. So yes this is the one and just to tell you so that your imagination will be easier is not that easy to imagine that how these lines are coming this is coming but that comes if I just draw a line, if I just draw a line yes if I just draw a horizontal line what is the meaning?

Student: (())(29:03)

Professor: That means I am now talking about at a particular conversion right, let us say 60 percent conversion how the rates are changing? Okay how the rates are changing see this is T starting from…normally we do not start from initial you know absolute temperature 0 but imagine that you are starting from absolute temperature 0, so what is the rate there 0 right. Then there is slightly more rate then slightly more rate then slightly more rate at that conversion any line horizontally will go through all this history right, so this is slightly lower, slightly higher, more higher then what is happening after crossing this again it is decreasing. How do I plot this? That means I have to plot this for a given conversion rate versus temperature how do I plot that?

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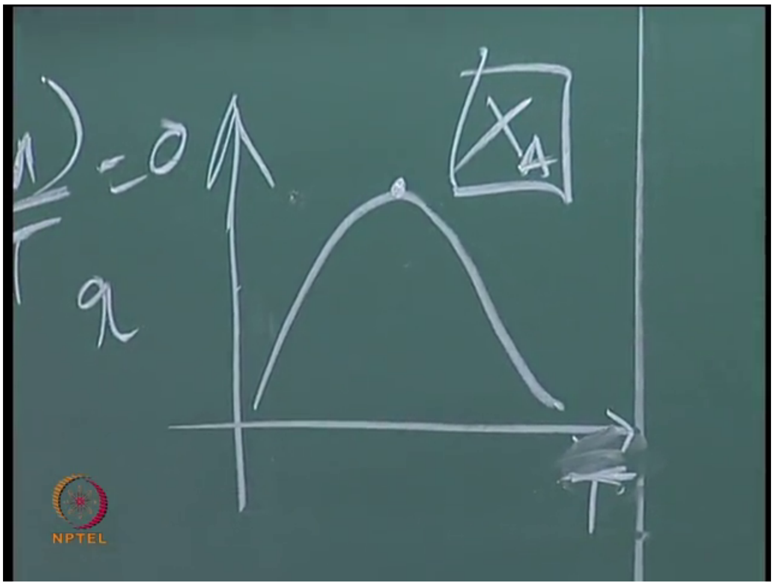

This is rate versus temperature, so how do I draw that?

Student: (())(30:13)

Professor: Yes so it may go I mean it may not be parabola exactly right. Then what is this point how do I get this point?

Student: (())(30:26)

Professor: How do I get mathematically?

Student: (())(30:29)

Professor: You cannot say D it should be doh why?

Student: (())(30:34)

Professor: All that is happening at 1 conversion x this is at X A constant correct? X A is the parameter, so similarly if I draw another line may be somewhere above right what do I get? About this I get or below this I get?

Student: (())(31:00)

Student: Below it.

Professor: Yes I mean if I draw this here.

Student: Below this.

Professor: Below that because these rates are definitely smaller than these rates if I go here this rate are much higher so that means lower conversion if I go to lower conversion that is what is reversible reaction because at high-temperature you get high rates but conversion will be lower that same thing only is reflecting there so then if I draw another line here and another line here so in which direction I have to (())(31:44) the conversion how it is increasing? From top to the…this is X A increase, so this is what we are telling you know these points are nothing but doh r by doh T equal to 0 and that is what is the line which you get now I thing is understood otherwise you know even last year also some people were asking Sir you are telling this but we are not able to get what is this doh r by doh T that is what is the line.

So there if I plot R versus temperature it is easy for me to tell I mean for you also it is obvious because doh r by doh T that is where what you are but here there is no doh r by doh T that means that this line is doh r by doh T but r is as a parameter that is coming there right but if you plot the same information in this X versus T now you have 3 para meters. Now I take at a constant r And then plot all that information then you will get this line maximum okay so that is why good, so this is the one. Now under these conditions what we normally do is our information tells us that go to the highest temperature that is possible because even though conversion is less what rate is high and in my design expression and I have this is rate in the denominator so I have to have definitely more if you want to get more conversion what you do?

You have to come back now, so that means maybe I am starting somewhere here right and it is again let us say adiabatic reaction that is the easy one so then you have going like this right but if I proceed like this this is the maximum conversion I get at my maximum conversion maybe somewhere here this is the conversion which I want okay or my design maybe 85 percent, 90 percent is the conversion which I want, so then what I have to do I will start as far as possible highest even I can start here it but where do you start is also optimisation problem T 0 what is the first T not otherwise the overall may not be optimal unless this is T not is optimal right.

So in this case let us assume that this is optimal and then yes it is 1 reactor this is one reactor PFR right so then I have reactor and then I have to now cool this till what point here it is very clear till what point we have to cool the reason is you will get this information from what is called the dynamic programming (())(34:29) is very famous for that he only give this conditions but (())(34:32) gave this condition what I am going to write a little bit later is the condition without mathematics by a simple logics he has written that condition because you know for optimality doh r by doh T equal to 0, so similar condition is also wrote for this optimality has been proved by later with people you know with actual mathematics okay that condition I will tell but because it is a there is no reaction in the heat exchanger this is cooling now it will go and stop only at this point because the rate is same, this rate line correct only one rate I have right.

On this it has to go stop only on this otherwise it is not economic okay but why logical common sense I think you know (())(35:16) had that one even without doing mathematics also he could tell that that it has to stop only on this reactor line and they did a lot of work on this particular exothermic reversible reaction particularly for catalytic reactions. Catalytic reactions we can definitely guarantee that the moment you come out of the reactor there is no reaction, so that is why you have to have the same conversion same rate but only temperature is decreasing because you are now cooling delta reaction mixture then you draw again parallel line this where you have to stop again depends on the mathematical (())(35:52).

Then you have this line right so then if you want this inversion again you have to go further maybe you have to just stop there okay it may not be economical but I thing correctly if you draw this and you will also go there and finally it has to be you know for optimality the general common sense is that we have to be both sides of this maximum this is this side this is this side. If you are only one side you will never get (())(36:26) right so the condition for this to be optimal.

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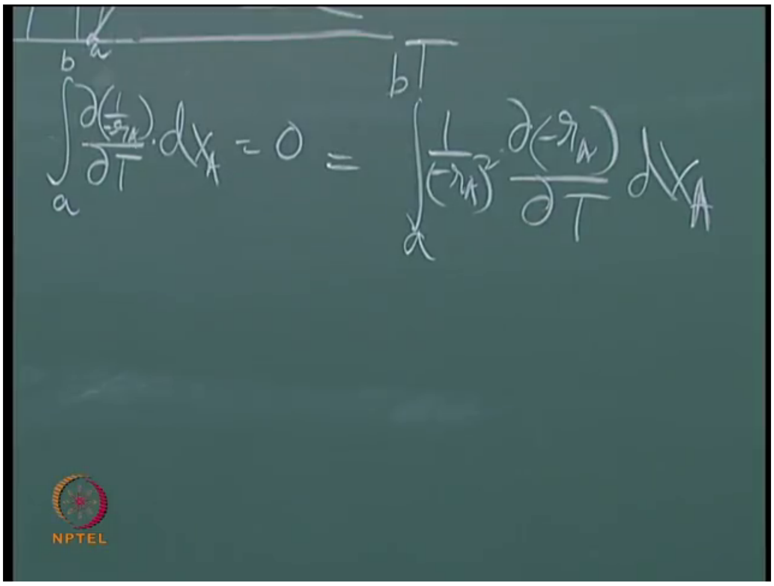

The condition for this to be optimal that means this (())(36:35) crossing this side is integral of course you have to be if I say this is a this is b doh of 1 by minus r A by doh T into d X A equal to 0. This condition you get from yes doh by doh T okay this is 1 by minus r A okay of course which also can be written if I just expand that this will be a to b 1 by minus r A whole square into doh T into d XA equal to 0 same thing okay so that is the condition.

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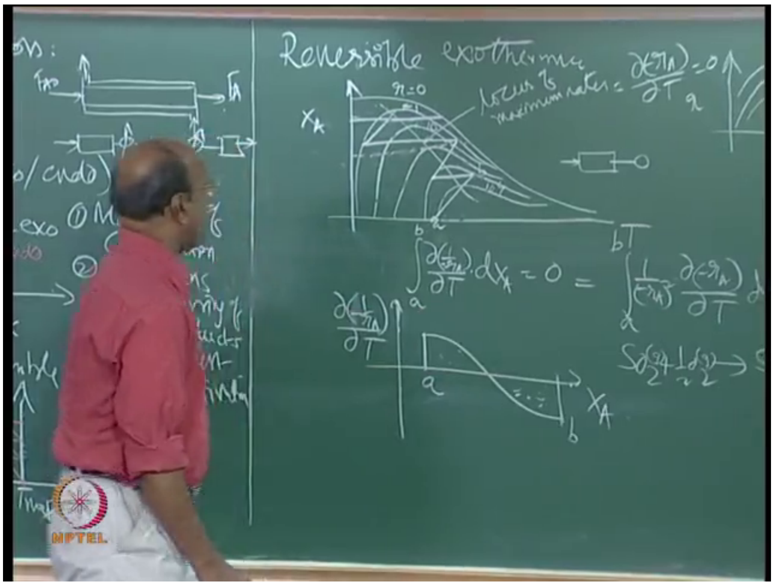

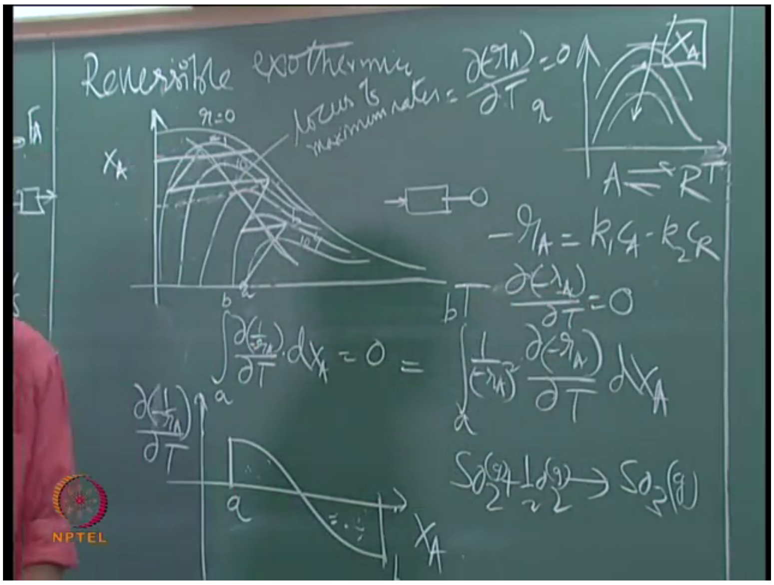

So in fact this one will be a condition where if I plot this one for example doh r by doh T versus X A okay I am plotting this, right. How it should be? Because the area should be 0 so that means somewhere it should be positive somewhere it should be negative, so it will be like this where this is a this is b okay, so positive area this area must be equal to this area so that is the condition.

So that means you do this try to find out the rates differentiated and then try to find out this area going on crosses goes and at this point you have to stop here if you are doing graphical, if you are doing by dynamic programming that will automatically fix that corresponding temperature okay good. So this is the one so that means this is exactly what is happening in SO 2 to SO 3 plus half O 2 SO3 this is gas, this is gas this is gas all gases and it is a catalytic reaction and they use adiabatic reactor. I will tell you why adiabators are used little bit later when you are coming to individual reactors okay adiabatic reactors are generally used if you do not have very high exothermic heat, so that means around 25 to 30 kilocalories per mole that is medium.

If you have 60 - 70 kilocalories per mole that is very high 60 - 70 kilocalories means that is highly exothermic right so almost isothermal you will get if you have 5 – 6 or 10 kilocalories per mole delta H r, I am talking about Delta H r okay so those conditions yes, so this is what is this and even this line how to get is simply differentiate this like what I have minus r A equal to simple reversible reaction k 1 C A minus k 2 C R doh r by doh T is k 1 is nothing but k 10 E power minus E by RT minus E by RT and k 2 also is simply K 20 E power minus E 2 by RT that you have to differentiate that I can give you in the examination this doh r by 0 okay yes I thing may be you have class.