Chemical Reaction Engineering 2 (Heterogeneous Reactors)

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Lecture 31

Graphical design of Fixed bed reactors

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Yeah, we have been discussing about the graphical design of packed bed rector first and then we thought we will go for the actual equations and the graphical design the other day I have given one graph I think I have written this graphical design of packed bed or fixed bed reactors, okay one graph what I have plotted was this right this is Xa versus T then I told you we have like this where rate increases in this fashion, no? Totally outer all are, I also wrote here minus ra equal to 1, 10, okay.

So like that this is one this is for reversible irreversible exothermic or endothermic that also we have written irreversible exo or endo you will get the same type of graphs when you plot, I mean conversion versus time T as parameter, sorry r as parameter.

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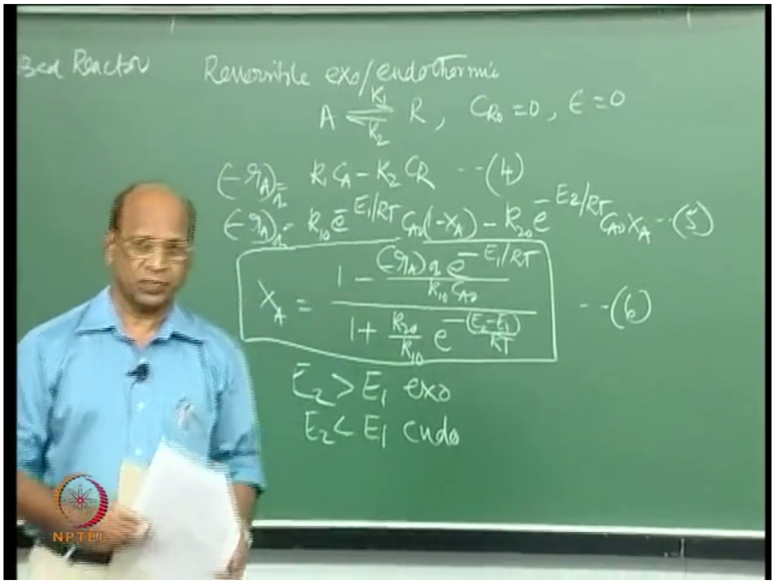

So we can also have we can start here reversible exo or endothermic for these reactions we have the equation let us say simplest equation I am taking but except the mathematics the procedure is exactly same A go into R we have K1 and K2 and minus ra can be written as K1 Ca minus K2 Cr here we also take Cr not equal to 0 that means it is pure A there is no R in the beginning, okay. So this equation can also be written as K0 K10 e power minus e1 by Rt that is for K1 and this also Ca not 1 minus Xa again assuming that epsilon equal to 0 again for simple algebra otherwise procedure is same then we have K20 e power minus e2 by Rt into Ca not Xa.

So this is equation 1, yeah did I give equation number for other one in the last class? 1, 2, 3 so this is 4, this is 5 this is minus Ra in fact here this is minus ra ob observed that means everything all the effects inside the particle also taken into account and then we are only writing in terms of Rob observed ray, okay still you can have this kind of equation for Rob also, right? Good. So this we will again separate to write in terms of this mathematics you have to do the same thing Xa I have to separating expression in terms of T, R as parameter.

So that if you do the algebra I think you are doing the mathematical work in the rooms (())(4:24) I can see a particularly quiz 2 paper I can see I think not able to do one I think not able to finish even the first problem which is very simple one writing on many many times you have written that, in spite of that that also many people not written in a proper way the first one you know where on the surface reaction equal to mass transfer equation Kg minus Kg into Cab minus Cas, yeah I think some people started writing the catalytic reaction you know (())(4:57) kinetics, yeah I think that means you are not understood at all, okay anyway how many times I can repeat, this is minus Ra ob e power minus e1 by Rt by K1 0 Ca not again whole thing divided by 1 plus K20 K10 e power minus e2 minus e1 by Rt, yeah, okay.

So this is the equation I trying to write this you can derive and this is equation 6, what nothing okay, so this is equation 6 this can also can be plotted yeah there is some more things here which you know your fandas I do not know whether you are still keeping them in your mind. So this e1 and e2 depending on these two values you will get either exothermic or endothermic which will be exothermic which will be endothermic, if Kavya e2 greater than e1 is exothermic, right yeah you will negative so minus delta Hr you will get, okay yeah so that also please write those who not remembering e2 greater than e1 is exothermic and the other one is endothermic, yeah so e2 less than e1 is endothermic.

So that means in this equation depending on that delta Hr value which is nothing but e1 minus e2, okay so you can also have that equation I mean that delta Hr here and then you can plot, right?

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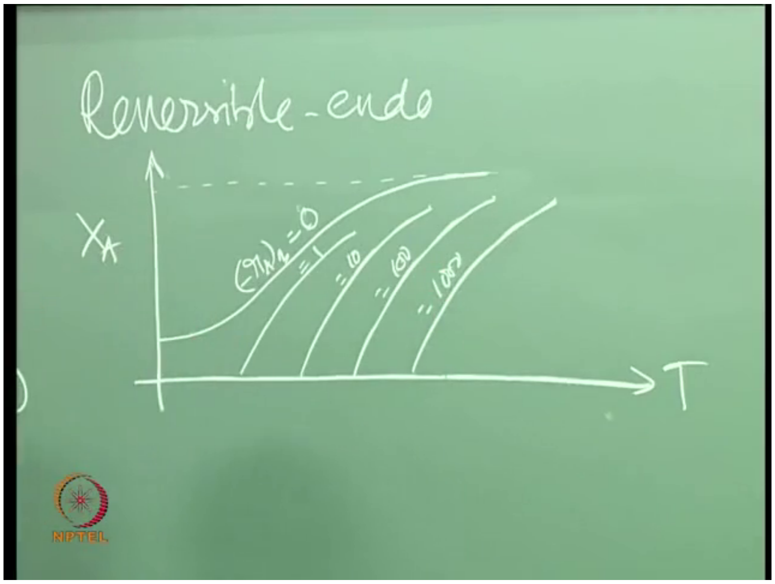

So when you are plotting for reversible endothermic you will get graphs something like this this is Xa versus temperature then you will have this is going like this this is minus Ra equal to 0 ra ob, sorry 0 that means it is equilibrium conversion, okay equilibrium conversion versus temperature at very temperature we will have corresponding equilibrium r equal to 0.

So then you can also have, for example r equal to 1, r equal to 10, r equal to 100 so like that so everything will be trying to go in that point equilibrium, okay so this is r equal to 1, 10, 100, 1000 like that, good.

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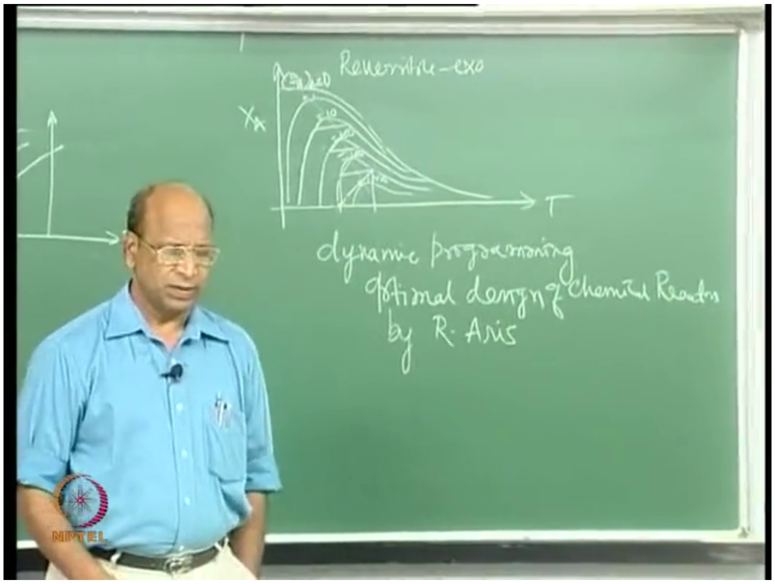

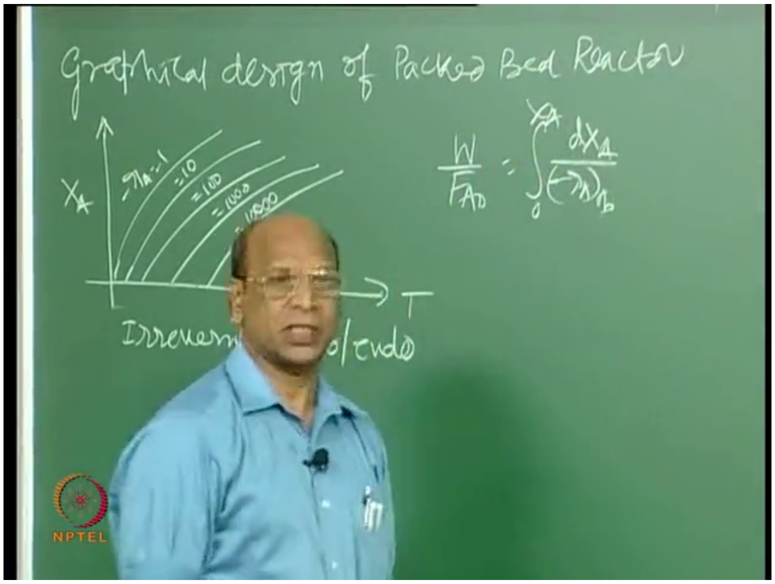

So for reversible maybe I think I will plot there I am using liberally all this board this is again Xa versus T and this is for reversible exo. So what you get here is very nice curve this is minus Ra equal to 0 something like this like this like this. So this is r minus ra ob equal to 0 this maybe 1, okay otherwise ra ob equal to 0 this is equal to 1, 10, 100, 1000, 10000 etcetera, okay beautiful, did you see Kavya this kind of graphs? Not so this is our again you know luckily the core companies are coming core companies they are interviewing you or it is only other companies asking how many brothers how many sisters how many fathers how many mothers, and correctly answering yes got the job, okay this is very nice information where many people ask that, can you draw the equilibrium conversion for exothermic and endothermic reversible reaction, okay.

So for exothermic, yeah reversible reaction conversion falls as temperature increases, okay equilibrium conversion, whereas for endothermic equilibrium conversion increases with temperature, okay yeah that is only to do with this equation where this is either positive or negative depending on this equation, okay. So now this is the information first we have to develop and this information comes from the simple minus Ra information minus Ra equal to some equation so that will give you this information.

So now how do I use this information for the design, right? This is very nice one. So that means in other words what I am trying to solve is the (())(11:20) and energy balance equation this is almost like our material balance equation and energy balance equation which gives me the relationship between Xa and T here also Xa and T that is the reason why we have plotted like that, see when you ar, yes no only what you are talking about is at equilibrium, okay but when kinetics come there is again you know it is reversible reaction where you have forward reaction and backward reaction till some point where you have the maximum here you will have the reversible reaction you know forward reaction dominating then reversible reaction dominating so that is the reason why you will have the maximum here and then falling later, okay that is the concept and you can also find out example this maximum, okay you can have a an equation again from this, okay that is, yeah dou r by dou t equal to 0 dou T because conversion is also is there Xa.

So when dou r by dou T equal to 0 all that you know maximum points also can be beautifully connected, so that means theoretically speaking we would like to be there on that point on this point, on that point why? Because there it is the maximum rate, okay it is not quite obvious here it is maximum rate if I plot the other way I can show you all those rates will be maximum, right? But here we are tracing this curve this reaches maximum and then it is falling but if I plot for example conversion versus rate or rate versus conversion rate is here then you can see that maximum but temperature will be another parameter, so that is why there is no doubt about that this is the maximum.

And that maximum is the maximum rate for me if I have all those maximum rates in the reactor because it is packed bed we said or you can take it as plug flow reactor along the length every cross section you have one rate, correct no? That is totally opposite to mixed flow why mixed flow as only one rate throughout the reactor that is the reason why we say that infinite number of times in series will give you packed bed because by definition of pluck flow itself it is infinite number of times because we are assuming the concentration along the cross section is uniform, okay that means uniform means like mixed flow reactor so each cross section is a see mixed flow reactor.

So like that you can put infinite number of CSTR in series you will get pluck flow. So that means at every point I have the rate and if this all those rates are maximum in my design equation rate is always in the denominator if all those rates are maximum then I will have the minimum reactor volume that is the reason why we can we should be theoretically on this point but that is not same if I go to endothermic reaction or the reversible endothermic reaction or irreversible reaction, irreversible reaction as temperature is increasing rate also is increasing, okay Prabhu for irreversible reaction as well as reversible endothermic as temperature is increasing you see the this one rate, so next if I go it may be 10000, 100000 like that it can go.

So what is the maximum I can use? That means I have to you see these are all very simple beautiful fundas I really get excited you know particularly with this graphical design, theoretically speaking here I can have the maximum rate that is possible to get the minimum volume so I should have one rate throughout which can give me the maximum rate and that will be in the denominator so you have you know w by fa not equal to integral dxa by minus ra, okay anyway let me write also once here we are talking about catalytic reactor otherwise it is V by Fa not 0 to Xa here we are talking about observed, okay.

So if this is maximum then my catalyst volume will be minimum and on the other hand if someone gives me this volume already this weight of the catalyst then I will have the maximum conversion these two are the design parameters always given the conversion find out what is the volume or weight of the catalyst or given the weight of the catalyst find out what is the conversion you will get the maximum conversion.

So that is why here there and here the maximum T max will be the temperature and that should be the isothermal that means otherwise you know that every point you have different you know rates the average rate also should be the maximum, so when can I have the average rate maximum? If you have all the rates are same, right? So like that what I have to do is I have to put infinite number of heat exchangers along the length of the reactor where everywhere I use corresponding temperature where I get the maximum rate, okay. So that is the reason why you can go to the maximum temperatures here, and what is limitation? Limitation is catalyst yeah (()) (17:07) of construction catalyst should not be spoiled so there must not be any side reactions beyond certain temperatures if you are able to take care of that you can go to any temperature, okay.

So that is why the optimum design for endothermic reversible reactions and irreversible exothermic and endothermic reactions is using the highest temperature where you get the maximum rate, if it is CSTR it is very easy even though we were talking about packed bed I can also cover that. In CSTR you have only one temperature and one conversion, right? So one concentration so correspondingly I can choose here for example yeah I can go some other like this and then say that for getting this conversion because conversion is fixed for us either you fix conversion and get the volume or you fix volume and get the conversion but most of the time for new reactors you fix the conversion and then get the volume.

So that is why if I draw the line, okay maximum conversion is that, so now for a CSTR it is very beautiful simple design because I have to draw the line where it goes through this particular point, correct no? There is another rate maybe this rate is going maybe that row this is the maximum temperature and this is the rate for this conversion so simply design will be W by Fa not equal to Xa by minus ra it is a mixture flow reactor, okay.

So again beautiful simply minus ra we will substitute there this value and then I will get the minimum volume or minimum weight of the catalyst. So packed bed is I mean the mixed flow reactor is very simple but here I should see that the average of all these rate should be minimum when I have the packed bed when I have the pluck flow reactor, okay. So that is I mean this and this is not that kind of exciting thing but here only it is exciting because you have to use high temperature high temperature definitely tells you that you will get higher rate but beyond certain point what happens is that rate will fall the rate started falling, so that means nowhere in the optimum sense I mean in the optimal region.

So that is why multistage reactor is used where you use one reactor to get that maximum average rate please remember average rate and then again you come out of the reactor put another reactor, right? Okay. So for example I can tell you that if I have a adiabatic reactor again simple one I am taking adiabatic reactor so then I can draw a line adiabatic line something like this when I cross this line it started falling because I am now going in the form of decreasing rates this is increasing all this is increasing rates whereas this side is decreasing rates, right?

So when I just cross this line then I will have I am going to have lower and lower rates which is not good for me so then I have to come back again I will come back I will explain this one to you later so like this see now this is the first reactor packed bed adiabatic system then from here to here I have to cool because this is temperature 1, temperature 2 this is temperature. So I have first a reactor then a heat exchanger then go to the next one I have another reactor next and then another heat exchanger here this comes through what is called dynamic programming where to stop where to start dynamic programming that is one of the optimization techniques dynamic programming of chemical reactors one of the famous books for this is by Aris optimal design of chemical reactors optimal design of chemical reactors by R. Aris this is one of the oldest books I think 60's actually that was his (())(21:22) thesis or so very small book beautiful very difficult to understand but I think worth a trying to solve that I mean use that book.

So here he has explained where to stop and all that I will also give you at the end what is the condition without understanding all that programming also we have some conditions where we can use so that we will get the minimum reactor volume, okay that I will give you later. So this is how you know multistage for example what is that sulphuric acid plants SO2 to S03 do you know that we use multistage fluid multistage packed beds there, do you know Lalita? For sulphuric acid plant when you have one reaction S02 going through S03 S02 plus (())(22:13) giving you S03, and what is the catalyst they use? This is the problem always all others when I ask one person x, x will not answer all others will answer, okay V205 correct, yeah.

So that reaction they use multistage bed usually 3 or 4 beds, so the reason is when you are going further and further here the conversion is falling maximum is conversion this is possible but maximum conversion you have here this is almost 1. So that means you have to start with higher temperature and move towards lower temperature you are moving towards lower temperature that is here you are again moving towards lower temperature if you have one more again you are moving towards lower temperatures.

So lower temperatures in exothermic reaction will give you more conversions, so that is why first you have to have at high temperatures start with then you have of course where you stop and all that this comes thorough this programing so then you start you stop here come back and the same because there is no reaction in the bed because in the heat exchanger because it is a catalytic reaction, right? So catalyst must be there to for the reaction to occur but in a heat exchanger we are not putting any catalyst it is simple heat transfer of the fluid I mean the reactant fluid reaction mixture, okay.

So that is why that is no problem so you can maintain the same rate again draw the same slope and that slope I will just quickly derive that equation so that I think they know already because last semester I have done and as I told you for if you take sudo homogeneous model they design what you learnt earlier in the reactor theory course this is exactly same this is same thing what we have discussed, okay because you are not at all trying to feel that there is a catalyst it is equivalent to your homogeneous bed where for homogeneous we have done all these reaction all these design we do not have to learn anything more but still it is my duty to remind you and also to repeat so that one more time repeating some people some more people may get, okay what is happening.

So that is why this exothermic reactions are very fast because as temperature increases conversion falls the other things are very simple, right? So now why should we get this kind of line and you know that mathematically also I will try to do that, yeah and okay this is also T max and when I want to be at this temperature where I get almost maximum rates, okay we want this is T max that means T max is only one temperature throughout that is isothermal condition even though many times we say that isothermal conditions never prevail but even here it they won't prevail but what really happens it is an endothermic reaction and it is adiabatic system we are not removing heat or adding heat here, okay that is the simplest design and industry people love to have adiabatic reactors, packed beds because adiabatic reactor again does not need any extra equipment you do not need any pumps again to send coolant, okay.

So not in one place sometimes you may have along the lengths 3, 4 heat exchangers that means one section with one temperature another section another temperature coolant in coolant out, okay if it is exothermic reaction if you want to cool. So all those things will not be there if it is adiabatic reactor, so that is why any decent industrial chemical engineer if he has a chance of using adiabatic reactor he just jumps and then takes, whereas that is not he not so lucky when you are talking about ammonia production, why? Prabhu any idea ammonia how they produce, what are the reactants? N2 plus 3HQ giving you yeah 2NH3, okay good that is nice yeah.

So then what catalyst they use? What kind of reactor they use, very good yeah what kind of reactor they use? For sulphuric acid I told you it is simple adiabatic packed bed they take the tube cylindrical tube and pack V205 vanadium pentoxide, but for ammonia it is not same, Anurag? (())(26:53) no, yea but what you mean by tower? Reaction tower means this also will be like this all are vertical in chemical engineering all are vertical horizontal nothing horizontal when it is not working, Anurag you have any idea?

How can we use CSTR it is a gas phased reaction for most of the gas phase reaction we do not go for CSTR, Abhinav? Kaviya? Kaviya can guess nicely, it is packed bed only because we have catalyst iron so definitely it should be packed bed, yeah exactly so that is why it is highly exothermic also that clue also I can give you, adiabatic they cannot use they know because they have to remove heat you know in again there are simple beautiful fundas there because here in SO2 to SO3 the heat of reaction is not that very high that is why they go for adiabatic whereas for ammonia reaction heat of reaction is very high they have to remove the heat.

So to remove the heat they use other do you inter stage cooling, inter stage cooling we are also doing in SO2 to SO3 multitubular reactor it is just like heat exchanger that is one of the very famous versions of ammonia reactor they take maybe 3 inches, 4 inch tubes and then put 3mm, 4mm catalyst, so like that they put all these tubes like exactly heat exchanger inside the tube you have the catalyst outside you have the coolant, shell side do you remember shell side, yeah tube side tube side is the catalyst shell side is the coolant and that coolant also of course it is just highly exothermic the coolant also is sent in the opposite directions so that you know that will be pre-heated your reactants also will be pre-heated all kinds of things wonderful designs are available there but you see because that is exothermic reaction SO2 to SO3 also is exothermic reaction but two different reactors we use because in one case that exothermicity is very high ammonia for example and in other case it is moderate heat of reaction.

So that is why it is not only the quantity whether it is continuous for very very large productions or small productions you go batch not only that there are other criteria also like I mean the heat removal if you have too much heat removal like packed beds particularly then you go for you know tubular reactors, okay then there is another thing also it is a gas phased reaction if it is liquid phased reaction highly exothermic and I have to control the temperature then I can go for CSTR and I do not know whether you heard of this or not fluidized beds behave like CSTR's fluidized bed is the you know that solid catalyst is made in the form of very very fine powder so I told you at one point where minimum fluidization where the entire weight is supported by the drag force so you will have exactly the ith some time back I explained to you also exactly the same fluid properties you will get for this solid, okay.

So that is why if it is still very very highly exothermic and temperature control is very sensitive they do not use packed bed they use fluidized bed, multistage if you want to go for more and more conversion because we know that mixed flow is very inefficient and plug flow is very efficient, why? Because of the concentration gradient only because throughout the system in fixed flow you have only one conversion that means you are not optimally using all the concentration, whereas in packed bed or plug flow you will have optimally using points at each and every cross section.

So that is why if you want if you have to use fluidized bed to control the temperature particularly one of the very beautiful example is (())(31:05) production (())(31:07) is very very highly exothermic, okay so all (())(31:12) reactors now operating in the world they are only based on fluidized bed, okay (())(31:20) also explains this and you know if you are not able to control temperature it will explode so that is the reason why they very carefully control the temperatures in the fluidized bed.

So there again mixed flow means I have the simplest design I do not have to draw this line I have to only see one particular point, how do you optimize mixed flow using dynamic programming again Aris has given actually earlier I mean we had so many courses optimal design of chemical reactors was one course packed bed reactors alone was another course, okay but at that time of course we had an M. tech stream called chemical reaction engineering so that is why we need more deeper and deeper so that is why we had but now almost you know jack of all master of none, so we tell everything in one class and then not able to concentrate much on that but definitely that will expose you to what are the basic things that are required for chemical reactor design I mean we need not feel sorry that we do not have that kind of so many courses this also if you concentrate you can learn so many things here, okay? Good.

So this is what is the graphical design and why we should get this kind of line I will also try to derive that now, very simple derivation I think this I can remove plus you are right, thank you how do you remember? Okay (())(32:47), okay good yeah that is plus only, very nice, okay anyway I am removing please correct that yeah.

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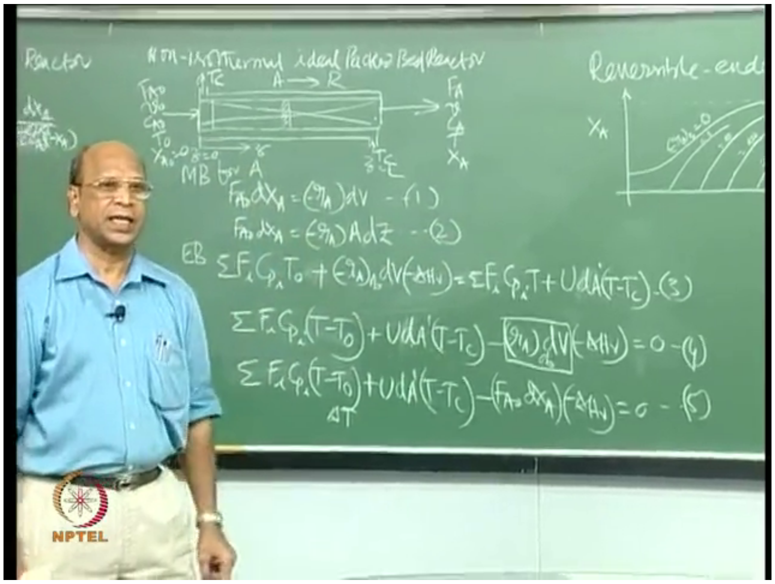
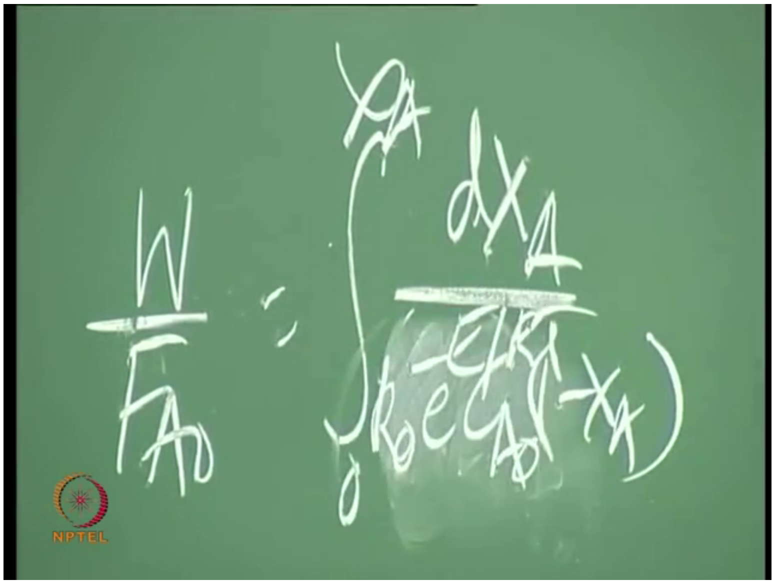
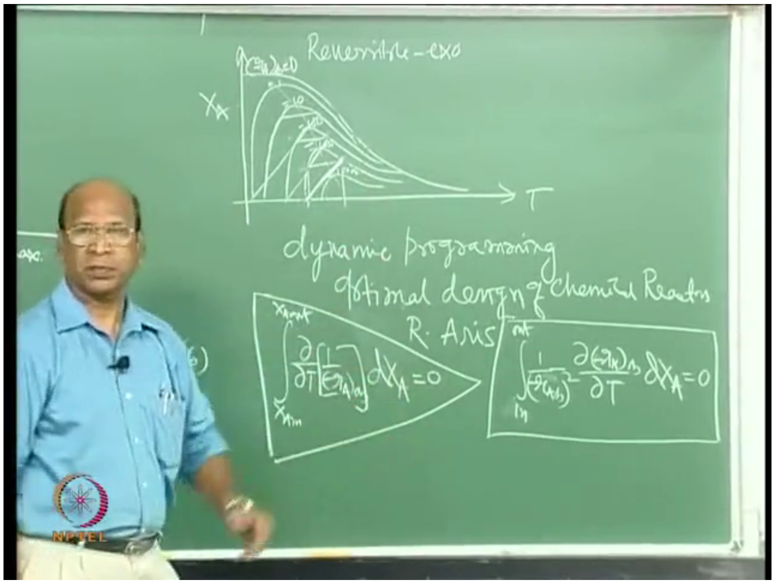




$$\frac{W}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{k_0 e^{-E/RT} C_{A0}(1-X_A)}$$



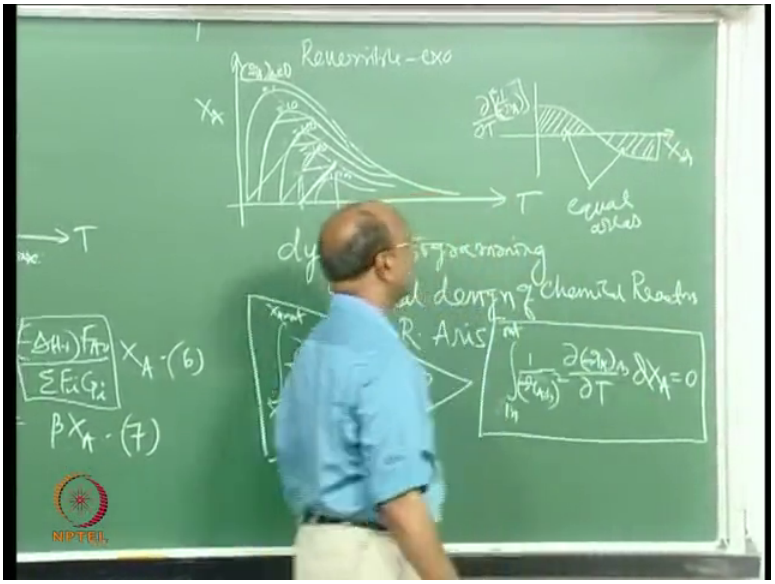
dynamic programming

optimal design of Chemical Reactors

R. Aris

$$\int_{X_{A\,in}}^{X_{A\,out}} \frac{\partial}{\partial T}\left[\frac{1}{(-r_A)_{avg}}\right] dX_A = 0$$

$$\int_{in}^{out} \frac{1}{(-r_{A,b})^2}\frac{\partial(-r_A)_b}{\partial T}\, dX_A = 0$$



This is let us say ideal p of r non-isothermal ideal packed bed reactor that means plug flow ideal packed bed reactor means pluck flow, right? So we have non-isothermal so we will have packed bed something like this we have packing everywhere so I have a heat exchanger like this, yeah this is coolant in Tc again to simplify mathematics that coolant never gets any temperature up, okay, why? Because its heat capacity is so large it won't feel at all, okay yeah.

So again Tc this is only for simple mathematics algebra to satisfy then we have Fa not V not Ca not T not Xa not usually 0 this side also you have Fa, v, Ca, T, Xa that cannot be 0, okay so I hope you know the meanings of that Fa is the molar flow rate moles per time and v is volumetric flow rate, okay and of course Ca, Ta and Xa all those things you know. So here if I take a small element inside for material balance, what we get is MB and I have a reaction as A going to R simple reaction, okay.

So MB for A will be this you already know so that is why I am writing quickly minus ra into dv, right? So this volume I can also take here in the beginning, okay anywhere I can take that, yeah this is one and yeah so this Fa not dxa can also be written minus ra this dv as cross sectional area A into dz if this is the z coordinate, so this is z equal to 0 here it maybe z equal to L that is the length of the reactor, yeah. So this is equation 1, equation 2.

So now for the same volume now energy balance I have to write energy balance for the whole components not for only 1 A, so when you are writing for that so you have sigma of Fi molar flow rate Cpi T not that is the total T not I am taking here because I am here I am writing there is a reason why because I can write this as delta t and each delta t delta x I can along the length of the reactor I can solve so that is why we are taking T not, otherwise you can take here and then put starting from T not onwards you can also do the things, okay that is input and this is exothermic reaction this is input, right? So this is exothermic reaction so the generation term will come this side because heat is generated so we have heat generation as minus ra ob dv minus delta Hr, right? This is nothing but moles per time dv and minus ra.

So that multiplied by so many calories per mole, so calories per time you will get there so this is the one this is equal to output, yeah okay sigma of Fi Cpi T some temperature here that is 1 plus you have UdA dashed T minus Tc, so I have written 1, 2, 3 here separately, okay. So you know what is this UA delta T term is this, yeah so this is the tube like this this is the tube we are writing from here there is an heat exchanger outside this is the area where the heat transfer is taking place that is pi into d, okay.

So that area we are taking pi into yeah d only, so that is this area into heat transfer coefficient and temperature difference and now you would appreciated why the Tc I have taken throughout same, in fact T will change Tc will change throughout along the length of the reactor but if I am assuming this this is same everywhere so correspondingly here T means T minus C, here T means T minus C, here T means T minus C T minus Tc, okay.

So that is why to simplify the algebra only we had put there otherwise you have to take that logarithmic you know your, yeah LMTD, LMTD you have to find out and that you have to substitute and it is a (())(39:08) procedure and it is very very because each time you have to find out for each section so that is the reason why we are simplifying and finally we have to check whether our assumption is right or wrong, okay but for understanding the theory this is the simplest one what we can give this is equation 3 then this also can be written there is a, yeah this can be written as this is the balance this is sigma of Fi Cpi T minus T not so this I have taken that side, okay so then we have this anyway as usual Uda dashed da is that area, okay T minus Tc minus minus of ra dv minus delta Hr equal to 0 this is equation number 4, okay.

So now we do not, this is obviously this is also obviously, okay but you know I do not like this term minus ra dv because energy balance what you have to get is the relationship between x and T, X and T I think I do not know whether B. tech students whether they have able to understand why we should write only in terms of x and T you know teacher would have taught you but I think probably you would have forgotten. See in here in this equation the simplest one if I take as K into Ca (())(40:55) reaction, right? So I have Ca not 1 minus x here and here also I have K not e power minus e by Rt, okay.

So now I have two parameters here T and Xa, what Lalita? This is an integral but this is with respect to Xa so I have to convert this in terms of either T or x one of them only one parameter I should have x and T x or T. So that is why I need a relationship between T and Xa so that this entire integral will be in one parameter one variable. So that is the reason why from energy balance I need a relationship between T and x here, right? So I can get that if this is replaced by this equation equation 1 if I put equation 1 here then I will have this is Fa not Xa.

So writing that sigma T minus T not plus UdA dashed T minus Tc minus Fa not dxA into minus delta H equal to 0, so this is equation 5, good. I can also write this one in terms of delta T, okay this as delta T this also delta x, right? And then I can of course I can try to solve that because it is only trial and error because you cannot have directly the solution, right? Otherwise if it is an because this T is also a problem for us, okay. So all that procedure I think last time I have explained but anyway now I want to tell you that we are talking about adiabatic reactor there adiabatic reactor design is the simplest and most useable design in the industry, okay adiabatic reaction.

So that is why which term I have to neglect here to get adiabatic equation? This will be 0 for adiabatic no heat exchange, okay. So then what is equation you will get in terms of T, tell me T minus T0 equal to for adiabatic case for adiabatic T minus T not equal to, yeah Fa not no minus delta Hr okay Fa not yeah Cpi and you have here delta Xa or Xa, okay, which is multistage? There is no multistage for any cross section any length it is valid that is no problem, yeah so if this is a constant we call it as beta T minus T not equal to beta Xa so this is 5, 6, 7, Cp? Is constant it is not changing with temperature they change but you know the moment you put that equation T square, T cube and all that impossible to solve this.

So that is why we see that how much it is variation between your limit of you know that temperature limits you have to calculate using thermodynamics you calculate your temperature reaction temperature maybe varying let us say 350 to 470 as an example. So within that is it very serious, if it is very serious you have to go for all complicated equations no chance, if it is negligible within our errors engineering errors then no problem we can use this analysis not only that even delta Hr even delta Hr also it can change with temperature but even that variation we have to find out within our operational regime whether it is serious or not, if it is very serious you have to take that all complication it is only mathematics procedure is exactly same it will be more complicated more messy in terms of equations that is all, okay.

So then if I plot this will I get what is the slope of this line? This is what I have been telling you is it beta just check, 1 by beta it is not beta because it is x versus T, T is y, okay sorry T is x I mean in our y equal to mx plus C that is what always I do not know who started first y equal to mx plus e I think throughout the planet we use the same thing I think for straight line equation, okay yeah. So if you want to convert in that fashion y equal to mx plus c then I have to plot only 1 by beta, so 1then by beta is this, okay beta is this 1 by beta is Fi Cpi by this one we are taking it is a constant and all the things I know Fa not I know total flow rates of all components I know then delta Hr I know thermodynamic quantity and then that if that I will draw the line here, 1 by beta and this boundary will tell me I mean theoretically I can go here but when I am going towards this what is rate here, 0 if you reach that 0 then what will be the volume here? Infinite.

So if you have infinite reactor (())(46:41) where do you stay and then operate, so entire universe is occupied by your reactor what you want to (())(46:49) no one can stay anywhere in the universe. So that is the reason why we cannot go to 0 rates, so you have to go only to certain limit and also as you go towards 0 rates your volume is becoming larger and larger and larger so all your money whatever you earned it will go for only designing the reactor because so much material you have to put, so that is why there is a limit for conversion in the practical sense, okay it can be 95 economically optimal conversion academically optimal conversion and no book will give you that for every plant you have to find out what is economically viable, not only every plant in every country you have to also find out because in some countries you may have materials cheaper in some other countries very costly so that is why every time when you are designing this economically viable conversion you have to find on your own depending on the local conditions, okay so that is why finally you have to make profit after at the end, good.

So that is why we just draw this line and there is a condition I do not know whether I have that condition here, yeah okay that condition is where you have to stop is integral Xa in Xa out dou by dou T of 1 by minus ra ob dxa must be 0, this is the condition, okay triangular 1 by minus ra dou by dou T of 1 by minus ra we can also write this in another form 1 by r square this also can be written as, okay in and out I will write it here now 1 by r square ra square ob square next one I am just differentiating this not er dou r, why dou r? Because Xa also is there as variable so this is equal to 0 same condition, okay.

So using that condition that means for example I can plot 1 by ra first, 1 by ra versus T I can take the slope at every point then I will have this, okay now that versus Xa I can plot you know how do I because it is not that easy to differentiate and get things if it is possible no problem because most of the reactions are not very simple reactions the way we have taken. So that is why you can plot 1 by minus ra versus T then take that slope at every point then that becomes dou of minus ra this is simply this is y for me 1 by minus ra is y, okay and T is x d by dx I am calculating, okay.

So then you plot this entire quantity again after getting all slopes versus Xa, right? So then you will have to see that this finally goes to 0 in fact that is also very very nice one where when you plot this you have to get so when I plot this whole thing dou by dou t of 1 by minus ra square, okay versus Xa it has to go to 0 no? No square sorry yeah, okay versus Xa if you plot how does the curve should look like? Finally what is that you have to get, 0 so that means you should have some positive area some negative area so it will go like this. So now you have to extend this Xa after crossing this slowly you have to count the area such that this equal to this equal areas, okay that is where you have to stop this that is the conversion where you have to stop this this is Xa I have written no, yeah this is Xa.

So very simply graphically we can do many many things and I think in the design problem last time or previously sometime last semester only no you have done this not all of you but some of you have done this, all of you? Only two batches out of ten batches, yeah. So that is how they have done and then they got very nice things but this is a wonderful experience but unfortunately this time design project is not catalytic reaction no it is a non-catalytic reaction, yeah (())(52:15) I have started doing Shekhar, so one day before the final thing, okay 2 days okay 2 days that is a great improvement from 24 hour to 48 hours, okay have you started reading at least the problem statement, what is the problem statement? Very good, stay in chemical engineering I say do not go to management do a one more degree in chemical engineering and then go for management but if you go to management coming back is difficult, okay it is not reversible so that will be irreversible the moment you go to management, anyway I am just giving you because so many wonderful things are there I say so many wonderful things are there what you can do particularly if you go abroad and get exposed to multi scale chemical engineering where I told you know last time where you can focus, can I focus only on the design of the catalyst particular or can I focus only on the crystal size of the catalyst you know first you have the crystals then crystals also have pores and all that like (())(53:28) then all the crystals will come as a solids.

So all the solids will keep in packed bed or fluidized bed and then all the fluidized bed are packed beds are kept in the plate, which scale you want to choose? You can choose the entire plant as your profession or only that one molecule how it is moving through the pores entire life you can spend there is sufficient things because still we have not understood quantum mechanics and all that.

So ultimate aim is can you say that to the molecule, okay now I will tell you move this side that has to move that is the kind of mastery you can take, no really that is how you have to control so then only you have the mastery over the molecules otherwise you do not have otherwise they behave like you behave, okay because whatever I tell in the class you never bother no whatever good things or bad things you never bother.

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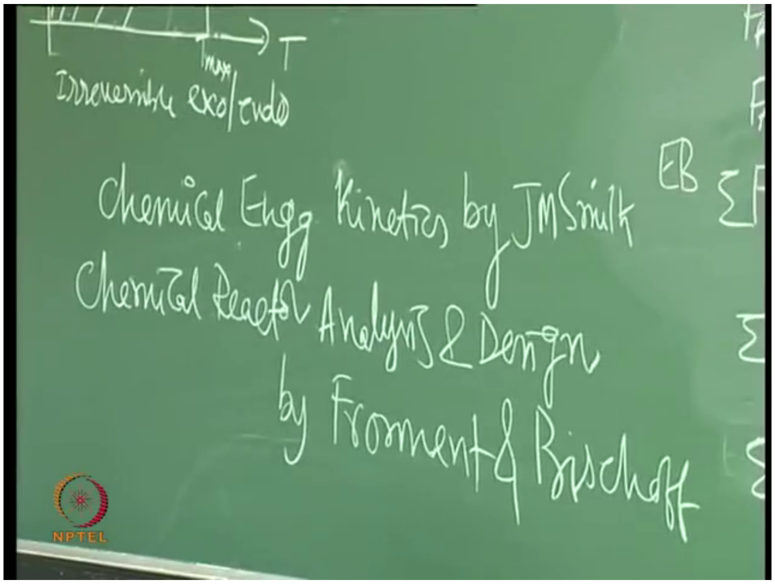

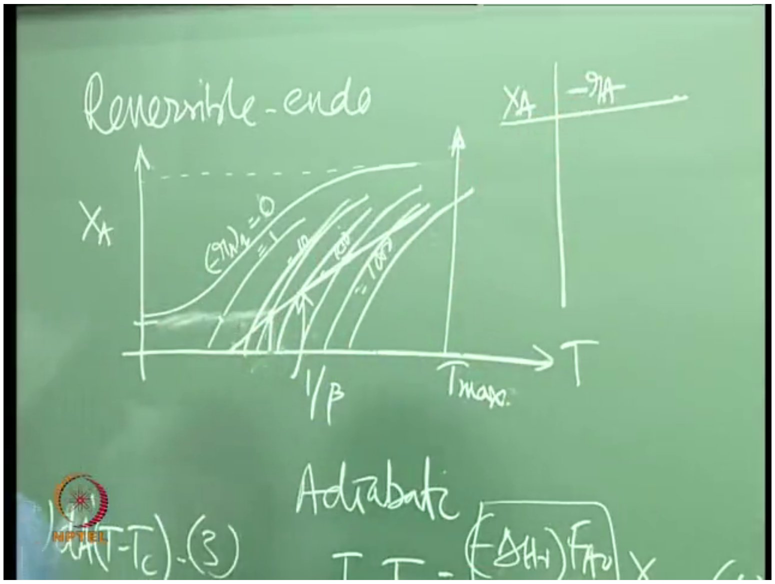

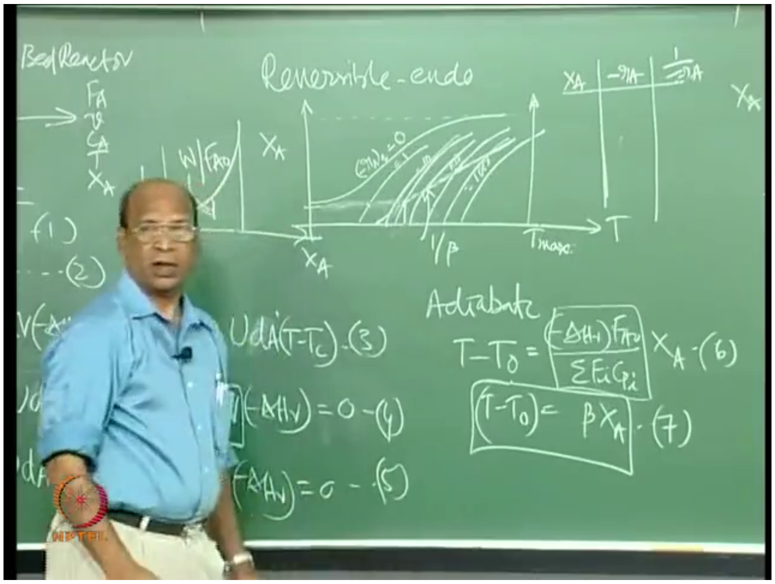

So like that molecules also I think if you are able to control then it is fantastic really very very so many wonderful things are there and also you know it is not that easy to design these reactors that is why I tell you first you see for the design chemical engineering kinetics by J. M. Smith, okay that is one book I think I will write make a note of this, yeah engineering I am putting short form chemical engineering kinetics by J. M. Smith let us make this fellow happy I say because he feels that no one is referring to his books, okay yeah but particularly thirteen chapter is the design chapter where he has, thirteenth no? Thirteenth or fourteenth you know thirteenth I remember but any way third edition I do not know whether it is thirteenth I think it must be thirteenth only.

So I think you know two dimensional model also he have mentioned not only one dimensional model he has actually solved step by step that is why I am not solving you have to solve you have to go through that book, the other book is chemical reactor, yeah can anyone guess? Not is (())(55:54) chemical reactor analysis and design this is by Froment and Bischoff, Bischoff is one of the greatest I think he died in USA and Froment is again one he (())(56:22) in the world and packed beds Froment you see they call him Fromo or something he is from Belgium, okay (()) (56:32) have some contact with Froment I do not know whether he is there or not but he has got some contact with this university he goes frequently there (())(56:40).

So Froment and Bischoff is another wonderful book highly complicated that means I know I told you chemical reaction engineering can be taught as simple as possible and also it can be taught as complicated as possible so you will never try to look at that subject later, okay. So that kind of confusion also we can make that is also possible but that confusion comes mainly because of the mathematics, same problems you know you complicate take an unisothermal take for example complicated rate equation highly messy algebra that is all nothing else, concepts are same even that complicated equations also they have to still use either plug flow or actual dispersion with plug flow or radial dispersion with plug flow like that only there is nothing.

So that is why these two books I think please see they are available in the library please go through that. So this is what I just want to tell you about the I mean graphical design, see I have only told how do you design but here also you can design if you do not want optimal design, optimal design means you have to go to the highest temperature but some design if you want to make it is not optimal you do not want to be at the T max but you can now take for example this equation for endothermic also it is same you will get the same equation then simply draw the line this is slope equal to 1 by beta, right?

So then what do you do it is very simple what you have learnt in your first class or second class maybe or cre 1, so what is that you learnt there if I have Xa versus yeah so here what I do is I will read now this is corresponding ra and this is Xa, okay and temperature also I have here temperature I do not need actually so this is Xa and then the rate here also Xa and then the rate and here, sorry here I do not want where this line cuts here it is cutting, here it is cutting, maybe there are many so many line in between so what I do here is Xa versus minus ra, okay.

So then I can also convert this into yeah 1 upon minus ra then you have again (())(59:14) plot wonderful plot, what is that? 1 by minus ra versus Xa so if you know exactly what is the conversion you have to stop then this area under the curve will be W by Fa not, same even here it same, okay this is exothermic reaction, sorry here I have drawn wrongly it is endothermic reaction no one pointed out also, okay endothermic reaction as temperature increases adiabatic no, correct? No no it should be in this line it should be in this way, yeah it should be in this way because temperature falls as conversion is increasing it is adiabatic endothermic reaction.

So this is again same thing procedure is same this point, this point, this point, this point, this point, okay yeah in that excitement I told the same thing for all three but this is the one this is endothermic you have the negative slope because as conversion is increasing it is adiabatic system that means no heat no heat removal or no heat addition as the reaction is taking place in endothermic reaction the temperature falls conversion increases temperature falls this is how it looks if it is a straight line, okay this is a wonderful thing (())(60:45) only could present this kind of wonderful points.

So it is there already in the maybe some chapter the third edition I am not very comfortable but in second edition its eighth chapter or so but you know this graphical design, graphical design is a wonderful design then I think tomorrow we will take the actual equations and then (())(61:05) ourselves, okay I will tell what are the equation that have to be used, okay then I think thank you.