

Chemical Reaction Engineering 2 (Heterogeneous Reactors)

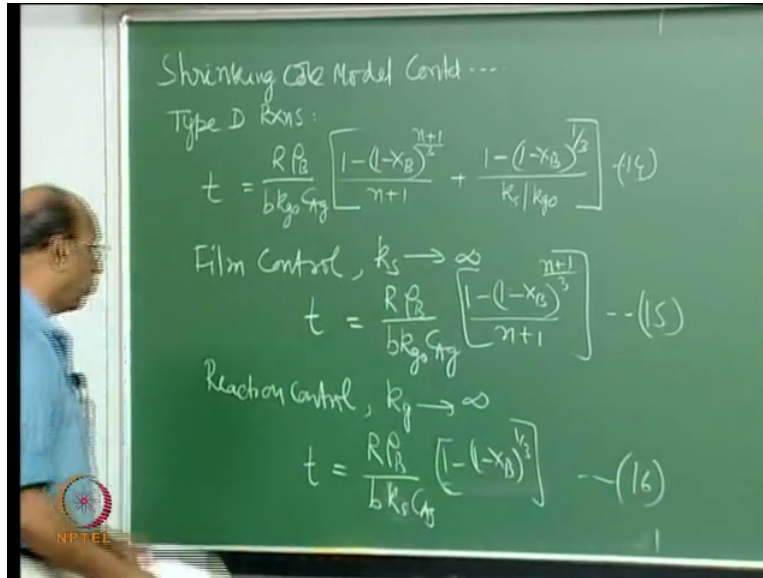
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Lecture 09

Shrinking core model continued for type D reactions Continued

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Ya yesterday we have been discussing about this particular equation where it is type D reactions where there is no ash or solid product on the particle so then we have derived this equation and this is the total time required for not total time this is the time required for certain conversion right, so if it is the two steps controlling that is mass transfer through the film and also reaction on the surface if both are controlling then this is the equation.

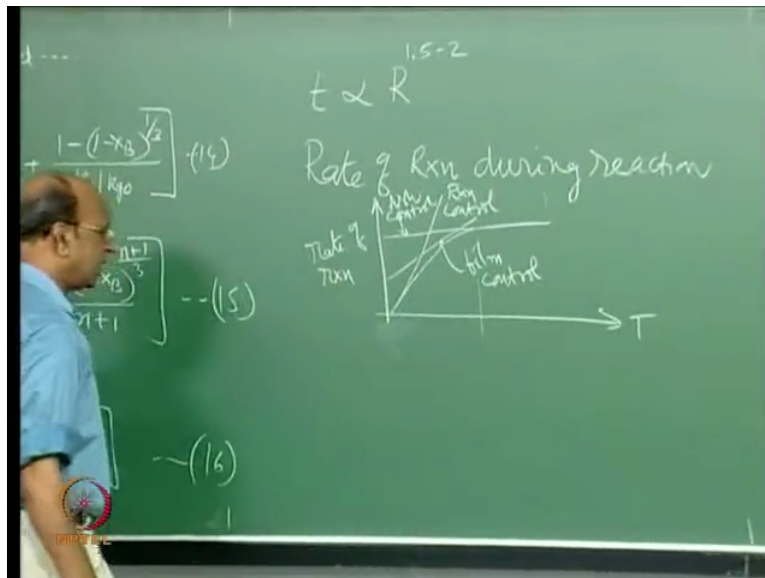
So as usual we can also now simplify this for individual cases if it is film control you know that k_s goes to infinity that means rate of reaction is very very large so then this term will not be there because this is 1 by k this k_s is very large so this term will vanish, then we have t film equal to $\frac{\rho_B R}{b k_g C_{Ag}} \left[\frac{1 - (1 - X_B)^{\frac{n+1}{2}}}{n+1} \right]$ this is the equation equation 15, then if I have reaction control and we know that k_g is very large value then the equation is t equal to $\frac{\rho_B R}{b k_s C_{Ag}}$ into only this term will be there so this will be $1 - (1 - X_B)^{\frac{1}{2}}$ to the power of 1 by 3 by (oh sorry) this will be simply k_s ya this will; be simply k_s ya so this is equation number 16, okay.

So if you look at particularly equation number 16 I do not know I think in your notes can you check what is the reaction control equation which we got for the other model where product

also is present on the surface ya it is exactly same no it is same do you know why it is same? Ya so the other steps do not you know even if they are there we do not feel at all so it is only the reaction control ya so the other two mass transfer steps are faster.

So then this is equivalent to your reaction control where you know the other mass transfer steps are not you are not seeing the mass transfer steps at all it is only the reaction control, okay. Whereas here it is not exactly the same and you can depending on this k_g value again this k_g changes with diameter, right this is what yesterday we have seen k_g changes with diameter and you know that for large particles it is inversely proportional, right and for large particles no for small particles it is inversely proportional and for large particles it is 1 by square root of d_p these two cases, right.

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So if you substitute that in this and then try to simplify then you will get this t is proportional to r to the power it depends on the small particles and large particles 2 1.5 to it changes the exponent changes to 1.5 to 2, okay ofcourse we can also calculate now what is τ τ is conversion for ya 100 percent conversion time required for 100 percent conversion then we can calculate τ and we can also write this is called as t by τ , right.

For example if I write this one as t by τ ya what do you get only this will disappear ya but n plus 1 will be correct no this will not go to 0, X_B equal to 1 ya and here right will be there X_B equal to 0, X_B equal to 1 it will be there. Now this n plus 1 depends whether you have small particle or large particle, for small particle it is (half) 1, for large particle it is half that will come there that coefficient will come there but that will be there, okay and this τ if I

take here this is straight forward only this much will be there, okay. So then in terms of t by τ also one can write these equations, good.

So you please just think about these things and with this the two models which I wanted to do we have completed and they are not very difficult models they are simple models and we wanted to make the entire process as a simple process without much complications and it is said that shrinking core model in most of the time most of the time it is valid for gas solid reaction, non-catalytic reactions.

But what can be the deviations in this model? When can you say that this may not be acceptable? Because no model is acceptable in all the situations, right 100 percent that is why we have some assumptions and all that ya which assumption may not be valid? The first assumption what we made was that you know isothermal I think it is a valid assumption because the particle conductivity is very very large. So generally when the particle unless otherwise you have highly exothermic reaction if you have exothermic reaction that is not valid because reaction is going on temperature changes ya but one thing which is not mainly valid is the sharpness of the shrinking core model, we have nicely drawn no one particle and this at centre after some time t we are just saying that that is the shrinking core that actually will be diffusive that actually will be diffusive.

So that means exactly your C_A is not there and r_c you can never identify exactly that is the sharp boundary that is one of the things but anyway I think you know people have done experiments and then finally found that this is one of the very well represented model for gas non-catalytic reactions, okay good.

Afterwards a few more things about this one some more information about this if I have the shrinking core model and as I have been telling you that we do not know which one may be rate controlling? There are various ways you know τ can be used. For example if you want to plot the whole rate versus temperature through all these things again analytical is some information must be in our mind, so I am simply trying to plot my rate of reaction versus may be with respect to A, okay or with respect to B right. So because the other one is nothing but $-\frac{dN_A}{dt}$, right equal to $-\frac{1}{b} \frac{dN_B}{dt}$ so that is only the relationship, okay.

So if I am able to plot either one of them how does that look like? Rate of reaction during reaction during the entire reaction you do not know which one is rate controlling, okay. So if

you have only one rate controlling atleast we can easily visualize but here what is that what we can normally expect is something like this. So this is rate of reaction and here let me plot with temperature that will give us an idea which may be rate controlling, right.

So you know logically you can also get the answer for this at low temperatures generally which will be rate controlling reaction rate, at very high temperatures mass transfer. So at low temperatures the rate may slowly increase like this okay and after sometime it may go like this this is one logical way of representing the rate of reaction with increase in temperature. So I can say here that I have this one is reaction control, okay ya here what is controlling ya which mass transfer I have two ya Ash is controlling.

So this may be ash controlling and in between somewhere you may have film control, okay and we know at very high temperatures even the mass transfer through the film may be higher when compared to diffusion through the pores ya ash through pores through pores. So that is the reason why this is the kind of curve we may expect and as a check if you do not have which one is controlling, right so let me say that you do not know and you did like this and you got only this portion that means you got all the time the straight line in the temperature you have conductor.

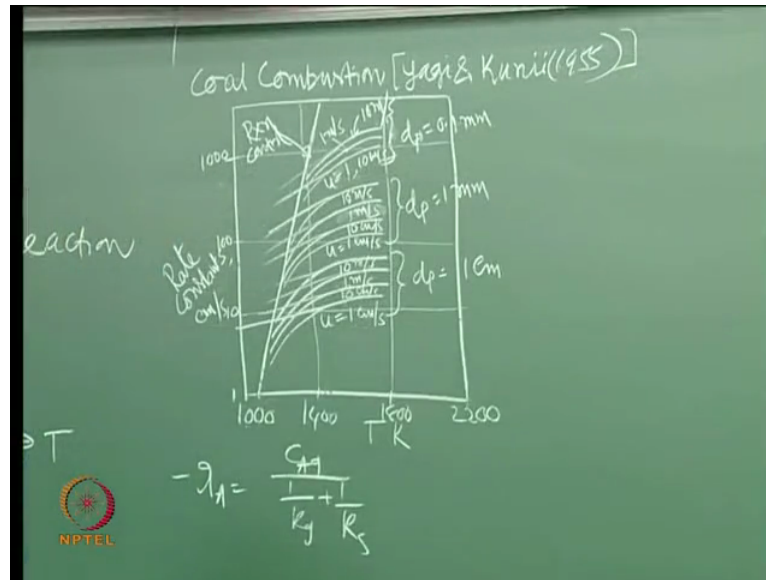
So then what is the idea you get? Rate of reaction and it is only going like this but it is not going you know taking this turn and becoming almost horizontal, no it is not happening it is only just almost a straight line, okay so then we can conclude that this may be reaction control and then here you do not get all this portion when you start at a high temperature because the temperature range anyway it is not theoretically 0, okay ya.

So at high temperatures and you do not know which one is controlling you are somewhere here, okay so at that time when you are getting almost there is not much change even though you are increasing the temperature it must be mass transfer control and generally in this shrinking core model it is diffusion control because diffusion through the pores is generally difficult when compared to diffusion through the film because film what do we have in film we do we have Shekhar? Ya it is only gas gas diffusion so it is not that difficult, right.

So whereas in the pores depending on the pore size if you have very large pores again that is a different matter that is what next we would try to do, okay for truly homogeneous model what kind of equations we have to derive but let me finish this whole thing about shrinking core model then we will go for that homogeneous model, okay so this is one and based on

this this first paper on combustion you know where systematic studies were done on coal combustion was done by some Yagi and Kunii in the Japan and they have very beautifully, systematically done even in most of you are not even born at that time 1955, okay ya.

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So how beautifully they have done the I think I have to plot here experimental so systematically coal combustion Yagi and Kunii 1955, okay. So he plotted or they plotted rate constants ya I think because it is actual data they have input you know centimetres per second and here it is temperature kelvin and how many rate constants will be there for coal combustion? Here how many rate constants will be there, rate constants in the sense may be you know all process including mass transfer as well as ya here only two but whereas in normal shrinking core model it will be three you know diffusion also comes there, okay.

And here we will have only two but you see how beautifully you know the data has been collected this is 1000 kelvin, ya 1400, 1800, 2200 kelvin ya this side the rate changes as 10, 100, 1000 okay this is 10, 100, this is 1, okay 1, 10, 100, 1000 it is a log log scale sorry ha it is semi log ya this is normal and this is semi log graph and then I will just draw the lines ya okay so then ya at 1000 slightly away from that starts and this goes to almost like this that is one line and then you have for if the diameter of the particle is 1 centimetre so then you will have it is okay I want to draw this okay (())(15:30) somewhere here okay so goes like this all this is for d_p equal to 1 centimetre and this one is u equal to velocity right yesterday also we have seen the term velocity there whenever deriving 1 centimetre per second, this one is 10 centimetres, this is 100 centimetres oh no no 1000 ya so this is 1 meter per second and this is 10 meters per second ya.

So then it is reduced to 1 mm, 1 centimetre to 1 mm so that will be again (16:35) draw this okay this is for d_p equal to 1 mm again here we have 1 centimetre u 1 centimetre per second, 10 centimetres, (100 centimetres) 1 meter this is 1 meter and this is 10 meters per second per second. So finally you also have for d_p equal to 0.1 mm ya 0.1 mm here the velocities are 110 both are same here 1 u equal to this is 1 also 10 centimetres per second and the next one is 1 meter per second, this is 1 meter and this is 10 meters per second ya.

All that I have patiently drawn just to ask you how to interpret the data okay in the examination I am very dangerous man you know in the examination I will give that graph and then ask you okay write about that, what do you predict that is very good training I say because that is what what you do in your P.Hd or in whatever you do research, okay you draw the graph collect the data and then try to interpret what is happening, okay.

So this regime is which controlling? Low temperatures, this is reaction control and here if I draw this line something like this, then like this something like this, something like this all all these lines ya so this line okay this line will give me the k value k_s value this one okay and this line will give me k_g value, right from here to here ofcourse these values are actually given by them these are all k values, okay these are all k_g values. But you see it is increasing like this, increasing like this and here the asymptote where truly I have the mass transfer control.

So the simple reaction rate for this is minus r_A equal to $C_A g$ by $1 + k_g$ plus $1 + k_s$ that is the one, okay. So low temperatures this is infinity this is controlling, high temperatures this is k_g is controlling, okay. So there are many things it is not simply I have drawn and then you know we will just close here there are many things what you can predict. So what is happening with increase in d_p or decrease in d_p ? The rates are increasing ya why these are the questions generally take d_p equal to 1 centimetre, 1 mm and 0.1 mm so the rate of reaction we say that it is increasing ya rate of reaction is increasing k_g increasing, what k_g should increase? As d_p is ya very good ya that is the kind of interpretation, okay we know that as you d_p is increasing or the k_g is inversely proportional to ya k_g the diameter so smaller the one more mass transfer so more rate of reaction, okay.

So within the velocities no you take one particle and now you see 1 centimetre, 10 centimetres, 1 meter, 10 meters so now again it is increasing is it logical ya ya so this is how one has to really present the experimental data so beautiful that is why even though it is one of the oldest one till it is very highly respected data, okay and I mean presently we do not

have that kind of patients to collect the data, we will take one point and write 100 models for that earlier it was reverse you take 100 points and then write one model because modelling easy now because you have computers, you have everything so okay and you have packages so one data point and then 100 models but older style is that 100 data points and 1 model which is staying all through because that is solid model, okay.

So this is how one has to find out really which one is rate controlling and how do you get the data all that information you can get from these graphs, okay and still the way I am explaining it is not that simple, okay you have never asked me how they have collected the rate of reaction data, okay for rate of reaction first and then only all these things are analysed or even here all that one has to really think before starting the experiment, how to analyse my data, okay I conduct the experiment but how do I analyse.

For example coal combustion data how do you find out? See we do not have thinking at all absolutely particularly with experiments, imagine that we have one particle and then I ask you to find out rate of reaction, how do you do that?

Student is answering: you can find the change of mass of the coal (22:54).

How do you find out? Correct I mean that is right you can find the weight loss, how do you find? So all these things you have to imagine no I mean no one is going to tell you if you get the job, Shekhar? So that is one thing I thought I will ask you you will ask me before that you know you just told on your own not asked, you know first of all you have two phases there, okay gas and solid which one you are concentrating, what Anurag was telling was that okay solid, solid also can be followed, gas also can be followed, right.

If it is gas oxygen concentration has to be monitored in the outlet but normally in the combustion process you send lot of oxygen and you do not worry so you may not have ya that is another indirect way of finding out, okay then you can convert into how much oxygen has been okay. So then what are the methods you use for analysing gas I am just trying to think you know we make you think ya if you do not have GC because people I think 100 years back or 70 years back I do not know they do not have GC, how they could have done it gas?

You have totally forgotten about this one no titrations totally forgotten no one is doing titrations nowadays I think ya that is like bullock cart technology you know that is solid all the time if nothing is working you know bullock cart will work because nothing happens to

bullock cart normally because there is no high fund of mechanism there I think to get spoil there, okay. So that is why this titration thing analysis is always valid but because we do not have patience that is why we are running after fast analysis ya GC is one I think now it is fair to accept that GC is one, anything else otherwise actually you have to do you have to collect the samples, take their samples and then dissolve in something else if you are following CO₂ take the sample or allow the outlet gas itself to go through some other chemical where all CO₂ is observed and then indirectly you will find out how much CO₂ is observed then you will calculate what is O₂ would have reacted all that, okay.

And okay as Anurag said I think if you want to find out the weight what is the technique used you heard of TGA Abhinav you heard of TGA? No you said TGA you did not say anything waving scale ofcourse the principle of TGA is waving scale only ya originally people have done that, they constructed very very sensitive balance and one side they used to put coal particle may be you know 10 grams or 20 grams or 50 grams and then the other side it is balancing the weight and you have I think in your I do not know whether you have done the drawing experiments that is one of the principles we also constructed that long time back, okay.

So then you can find out what is the weight change and you know that weight can be converted into moles and ofcourse moles per unit time and then you can find out what is the rate, okay. So all these things we do not normally tell all these things we do not normally tell it is exactly like our movies you know where I think I have been telling this no I think last class also I have would have told this.

All our movies how does the movie start, with young boy and young girl and then first either fighting or I mean first side they never fall in love even though they fall in love I think egoism they do not accept. So that is why the boy has to pay in the girl, girl has to pay in the boy and then till interval it will go over after interval I mean in between we have some songs and all that I think overall that.

So after that only Villain comes Villain may be in the form of Mother, Mother in Law for you know both sides, or Father, Father in Law so like that you know Brother, Brother in Law, Sister, Sister in Law so you have in India so many relationships so you can that is the variation in all our movies, on movie will have brother, another movie will have sister, another movie will have () (27:06) also, okay. So all kinds of people you will have.

So then anyway after that I think everyone will accept and then the movie ends with marriage that is all what we show, all the problems actually starts after marriage. How many of us I think really seeing those movies this is also exactly like that we know we think that you know we are not telling you all that simply I plot rate versus concentration, rate versus temperature, right.

But if you do not think properly in your life you never understand what is that rate, how do I get this rate? That is why I told you even after P.Hd can you design a pump? Because we would have never told you how to design a pump, you could have solid problem, absolutely no problem, right you should have solid problems you could have got (())(27:52) out of that you know in that subject.

But finally when someone asks that okay I think I have a problem I do not know how to calculate by (())(27:59) means I do not know how to calculate that is why I made a point that you know every time I will repeat these examples, okay so that atleast you will be aware, you may forget the moment you cross the door you may forget okay like that Matrix movie where he tells that okay you do not remember anything the moment you cross the door. So I am not cursing like that but I think atleast you know most of you do that you will forget and you remember only just before one day before the examination and the next day you will again everything will go, good anyway.

So that is why there are so many things when you are teaching a course which is not directly told like our movies only I am telling, right there are so many so many things which you have to really remember, which you have to understand and for every course general thumb rule of Professor Anand is if I am teaching 1 hour you have to work 4 hours atleast in your room for that course, that is why we have 24 hours per day and maximum 6 subject so 24 hours that is the idea, okay per semester, okay.

So otherwise you do not get anything you can come and sit and look at me very sceptically this fellow talks something I think you know I just listen and then otherwise while coming I will a drill hole from this side to this side so that there is no retention there straight away it comes out, okay why you are wasting time. So that kind of attitude if you come and then you just stare at me that is all, otherwise I think at the end you do not get anything, at the end I do not get anything that I have a satisfaction that (())(29:24) them where they have understood something and then retained something, retaining is very important for teacher otherwise I

think next year semester also if I teach all these things you come and sit here as if you never heard of this, okay.

Ya so that is the kind of teaching what we have and also your response, anyway we will close here Monday Monday only no Monday we will meet and Monday again I can give for example derivation of this, okay.