Chemical Reaction Engineering 2 (Heterogeneous Reactors)
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Lecture 06
Shrinking Core Model Continued

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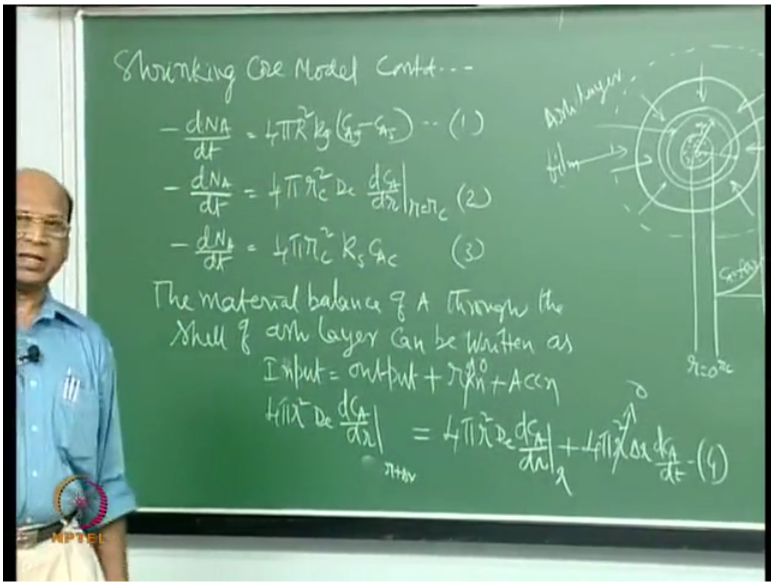

Shrinking Core Model Contd...

$$-\frac{dN_A}{dt} = 4\pi R^2 k_g (C_{Ag} - C_{As}) \quad \cdots (1)$$

$$-\frac{dN_A}{dt} = 4\pi r_c^2 D_e \left.\frac{dC_A}{dr}\right|_{r=r_c} \quad (2)$$

$$-\frac{dN_A}{dt} = 4\pi r_c^2 k_s C_{Ac} \quad (3)$$

The material balance of A through the shell of ash layer can be written as

Input = output + $\cancel{r_{xn}}^{0}$ + Accn

$$4\pi r^2 D_e \left.\frac{dC_A}{dr}\right|_{r+\Delta r} = 4\pi r^2 D_e \left.\frac{dC_A}{dr}\right|_{r} + \cancel{4\pi r^2 \Delta r \frac{dC_A}{dt}}^{0} \quad (4)$$

Now we will start deriving the continuous I mean we will continue shrinking core model derivation. We have written three equations that again I will write here for connectivity equal to 4 pi R square C As this is 1, 4 pi R c square ya De at r equal to r c this is 2, again 4 pi r c square k s C Ac this is equation 3. So now our general procedure is to eliminate the intermediate concentrations and then express this in terms of only measurable quantities like k s, De, k g and this concentration that is the usual procedure, right.

But here we have a problem we have dC A by dr where I cannot easily eliminate using like C Ac and C As. So we have to develop an equation for dC A by dr in terms of C As and C Ac, right. So that means we have to have a concentration profile C A versus r r is the radial distance and then you differentiate that and evaluate at r equal to r c then you will get concentration C Ac and also C As, right.

So using that you can eliminate the intermediate concentrations so now the question is how do we write how do we derive an equation for C A the concentration profile of A through the ash layer, right okay.

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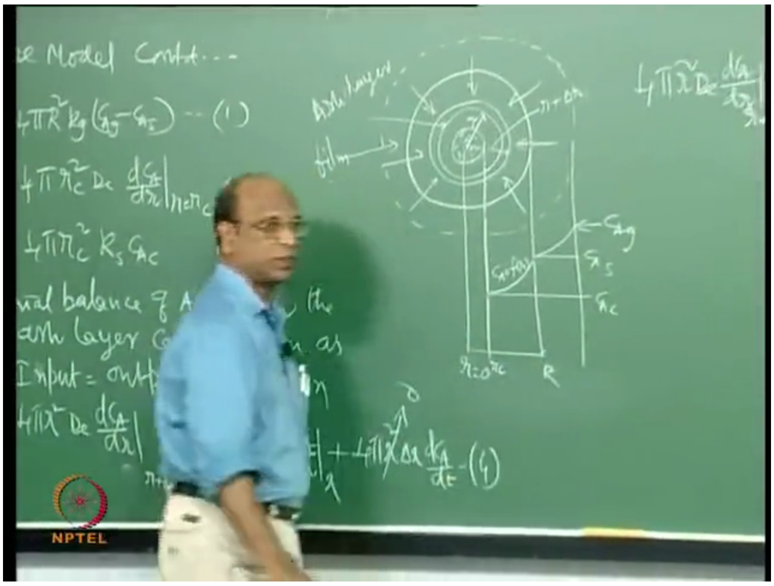

So that is why we first draw this picture for ash layer so this is the particle, then we have here B that is the shrinking core actually and here we have the film so this is centre, this is r equal to 0, I have capital R here ya so then we also have r c, this is capital R ya so if I plot the profile which we have many times this will be C As and next one will be ya this is C A as a function of r and here I have C Ac this is the profile what we require, if I have this profile then I can differentiate and evaluate either at r equal to r c or at r equal to capital R so that is okay I mean that is left was whichever is convenient we can do that. How do we do this?

That means when A is diffusing from surface to the core through the ash layer, ash is inert there is no reaction so it goes as if there is an inner porous body through which A diffuses, right. So we have to write the diffusion equation for A going through ash layer, okay let me also write that this is ash layer ash layer and ofcourse this is film, okay. So now through the ash layer when you are writing the equation again I have to identify a shell like for example this one ya so what we do here is we have from this is r and this one is ya r plus delta r okay this is r plus delta r so that the thickness is delta r for me, good ya.

Now how the diffusion is taking place? Diffusion is taking place all through like this, okay may be just we draw few that is the diffusion that is going through A, right able to follow, okay ya. So now I have to write what is the amount of A that is diffusing through this line that is the shell actually, shell boundary through that that means through r plus delta r then it is coming through this then I have r and what is the rate of reaction? Is there is rate of reaction or accumulation, right.

So mass balance for A I think we better take this one the concentration gradient in equation 2 the concentration gradient in equation 2, dC A by dr at r equal to r c can only be evaluated if can only be evaluated if the concentration profile is known through ash layer through ash layer. The derivative of the concentration profile at r equal to r c the derivative of concentration profile at r equal to r c will provide the equation in terms of C Ac and C As, C Ac and C As, ya.

So then the material balance the material balance of A through the shell of ash layer ya can be written as can be written as okay input input equal to output plus reaction plus accumulation I am using the short form. So reaction equal to 0 for the reason that ash is inert and there may be accumulation through the shell and if I write this, this is diffusion so it is only Fick's law right diffusion through the shell.

So that is 4 pi r square De dC A by dr at r equal to r plus delta r okay that is one okay I think r equal to I do not have to write let r plus delta r this is also equal to 4 pi r square De dC A by dr at r that is output that is coming out, okay input, output and reaction equal to 0 and accumulation is ya 4 pi r square delta r dC A by dt ya I think actually I have to write dou here okay ya but anyway I may not writing dou there because I will tell you that one of our assumptions is pseudo steady state, okay.

So that means I have this one pseudo steady state means there is actually steady state but it may not be pseudo but why we call that pseudo steady state I will explain so this also we will take it as 0 based on assumption of pseudo steady state, okay I will explain to you what is pseudo steady state later, right okay. So this is the one please see that in the equation this is equation 4 accumulation term is neglected based on the assumption of pseudo steady state theory, right.

So what do you mean by this pseudo steady state theory I will just explain and mathematically also we can prove that later. So this is the one, what is our idea we have to evaluate what is the concentration here and also what is the concentration here so that I can now use those two concentrations in this equation and eliminate C Ac, C As and here finally express in terms of C Ag, okay that is the idea.

So now when the diffusion is occurring, reaction also taking place when reaction is taking place this core is moving that is going inside. So when it is going inside then I do not have a fixed boundary correct no this is fixed anyway here diffusion is taking place (())(11:56) got integrate from here to here r to r c but r c is not constant r c is continuously moving. So the pseudo steady state assumption state says that if I have the diffusion velocity through this ash much much much faster than may be thousand times faster than this shrinking core velocity, core also is shrinking so if that rate of shrinking should be thousand times smaller than velocity of diffusion, if that condition is satisfied then practically what happens at any time when the gas is coming this is practically constant that is what is pseudo steady state and this condition can be easily used for gas solid systems because the gas diffusion through porous layer is much much faster but this condition cannot be used for liquid solid systems.

Like for example it can be a liquid you know in ore leaching ore leaching also is done you take a ore and then put sulphuric acid or hydrochloric acid now this hydrochloric acid has to go inside and then react. Now the diffusion of this hydrochloric acid through that is not that fast when compared to core. So under those conditions we cannot assume pseudo steady state for liquid solid reactions, why? Because the densities are comparable whereas the density of gas and then density of solids will be thousand times, okay ya.

Anurag do you have any idea what is the density of air at room temperature? Anurag is only 1, okay this is normally the problem in all classes no when I ask a question X, X will not answer all other people will answer, okay ya and for solids normally can vary a lot, for sand what is the density? Because every day we see sand (())(14:12). Prabhu you have any idea? Density of sand? May be around 1000, 2000, 1000 or 2000? (())(14:25) means ya Kavya you know?

Student is answering: 1400 to 1500.

1400 to 1500 come closer ya Rinita? 1600 it is like auction, okay we going higher and higher it is 2600 this is what is unfortunate with most of us because as engineers we cannot really estimate you know we will not have anything in our mind about some values like for example what is the diameter of this chalk piece? (())(15:03) 5mm, half an inch I am happy you have not told one kilometre anyway ya so that is what is the meaning of this pseudo steady state I think you know in every simple terms I am explaining that, okay.

Our idea is to again correctly get what is C Ac on the surface if C Ac is I mean okay if this core is moving C Ac also continuously changes but under pseudo steady state conditions the velocity of diffusion of this gas is so fast at any time this profile is established at that instant of time. So that means this is constant at this instant of time, it is not moving but whereas if the velocity is diffusion velocity is smaller comparable with core receding velocity then you cannot assume that, it is exactly like you know there are many beautiful this is called moving boundary problem, okay there are many beautiful problems like one problem is your eyes you know when you are taking a drink you put ice know.

How the ice boundary is slowly moving? There is heat diffusion right otherwise it will not melt know ya so that problem also is solved using not pseudo steady state theory but you have to take the actual this term also into account mathematically it will be complicated but particularly for gas solid reactions this will not come into picture we can prove that later because normally it happens if the density of that is why I was asking.

So typically if you have either 1000 or may be 2000 or sometimes 4000 for solids like you know iron ore and all that iron ore density will be around 4.8 iron ore, okay so we are using also iron ore for the (catalytic) non-catalytic reaction, right what is the reaction to make ore? Ya what is the reaction? So many times I have written the reason, iron ore ya Fe2 ha ya good balance you ask me to do those numbers, okay anyway I am happy atleast you could tell that this Fe2O3 is it magnetite or hematite? There are two ores no why (())(17:25) ya why you say hematite? I remember always H comes first so Fe2O3, afterwards Fe3O4 magnetite, okay anyway.

So this that is also one of the reactions where the density is 4 or 4.8 also so that divided by 1.2 will give me again you know 2000 times also. So that is why most of the times it is very well valid but it is also not valid if there is very high pressure gas solid reaction, if the pressure is very high you know again density p is ya Prabhu what is the equation you said for density? Ya pm by rt, so the p is very large for high pressure reactions then rho becomes very very large if it is 100 then again it may not be you know 1000 times even with 2000, 3000 if you take so that is the reason why it may not be valid, mathematically also we will prove that after some time, okay.

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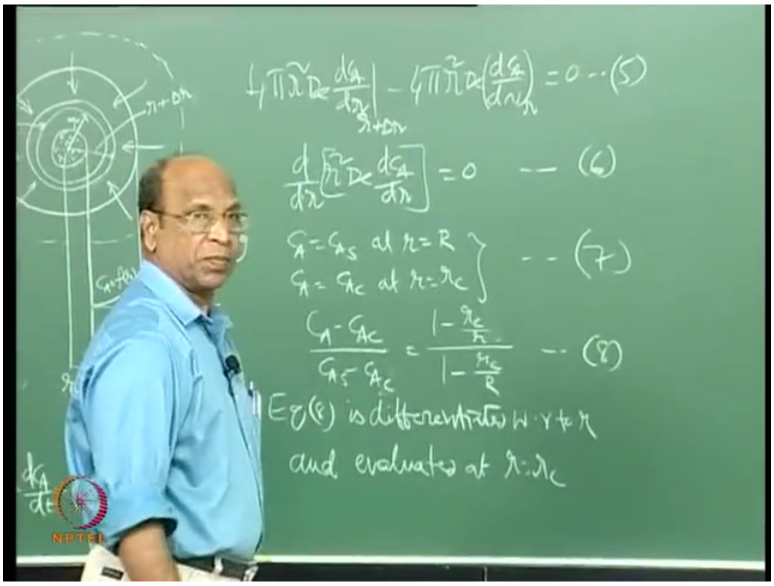

So now when I take this equation equation 4 and this is 0 and that can be written as 4 pi r square De dC A by dr at r plus delta r minus 4 pi r square De dC A by dr okay at r equal to 0, no one asked me why I have not put a minus there, only I have to answer questions and I have to question myself and also give the answers this is equation 5 ya. Why I have not put minus there? Here no normally the diffusive equation will have minus know, why Rinita any idea? Rinita is only one you are not Rinita excellent JEE solution all of them are minus you do not have to write, no there is a wonderful physical significance for that.

By the way why do you write minus there? Why do you write J flux equal to minus De dC A by dr? What is showing negative side?

Student is answering: Diffusion.

What is negative there? ya I mean I know you are now searching for words but may be you understand ya tell me.

Student is answering: The way we define the coordinates is.

Ya but what is happening? The concentration how the diffusion takes place from high concentrations to low concentration or ya but how do define differential? Ya because you know it is always we remember y2 minus y1, right. So but I think this is a physical quantity which cannot be negative flux. So that is the reason why we put minus there to take care of dC A by dr which is negative derive we define mathematically.

But here you see my coordinate is increasing in this direction, right and it is in the opposite direction, what we write diffusion so that is why we do not write not simply everywhere minus and then I cancel it, okay it is the coordinate system which I have chosen here, it is in the opposite you know the diffusion is in this, my coordinate is increasing in this direction so that is the reason, okay anyway.

So this equation if I write in terms of differential form r square De equal to 0 so this is equation 6. So now this has to be solved to get the concentration profile so now I need two boundary conditions, what can be the boundary conditions here C A equal to C As where at r equal to capital R, C A equal to C Ac at r equal to r c ya small r c so these two is equation 7 I am not giving the solution as I am not showing the steps of the solution.

And if you are able to integrate this twice and then substitute the corresponding boundary conditions what you get is C A minus C Ac C A minus C Ac C Ac equal to 1 minus r c by small r divided by 1 minus r c by capital R or for uniformity I will also write here divided by so this is the equation, right actually the concentration profile which I draw here can now be plotted if I know these values C A versus r okay that gives me exactly the shape whether it will be like this or whether it will be like this, okay that gives me the correct mathematical ya from this mathematical equation we can also draw that. Provided I know what is r what is small r c and C As and C Ac, C A versus r we can plot that, okay good.

So now this has to be integrated sorry equation 8 has to be differentiated and evaluated at r equal to r c, okay. So now equation 8 differentiated with respect to r with respect to r and evaluated at r equal to r c, okay so this I will give you in my surprise test but then what you get equation is okay.

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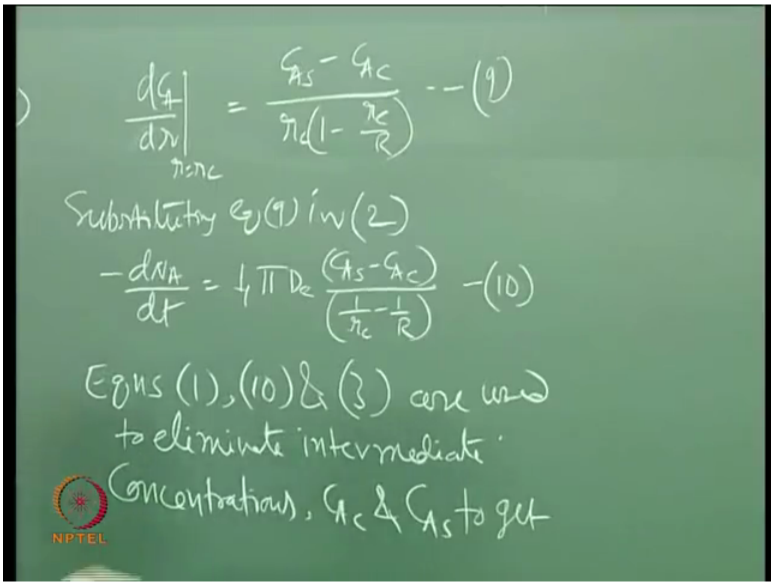
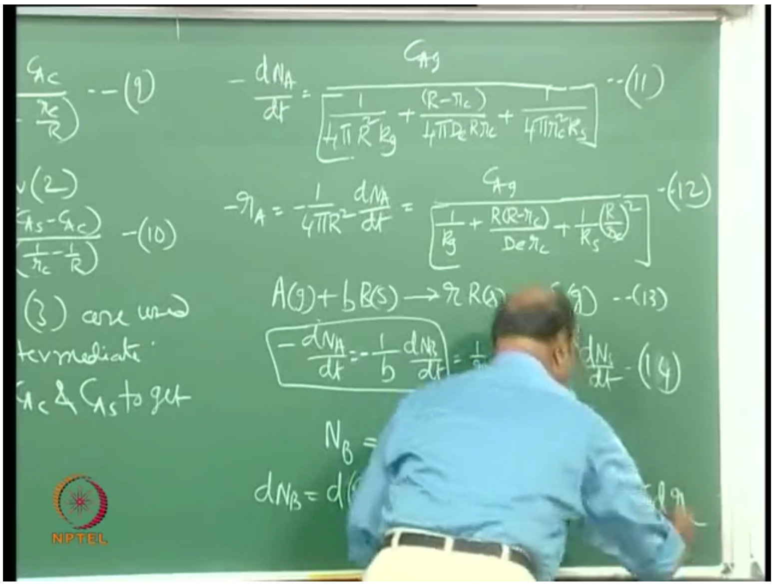


$$\left.\frac{dC_A}{dr}\right|_{r=r_c} = \frac{C_{As}-C_{Ac}}{r_c\left(1-\frac{r_c}{R}\right)} \quad --(9)$$

Substituting eq (9) in (2)

$$-\frac{dN_A}{dt} = 4\pi D_e \frac{(C_{As}-C_{Ac})}{\left(\frac{1}{r_c}-\frac{1}{R}\right)} \quad -(10)$$

Eqns (1), (10) & (3) are used to eliminate intermediate concentrations, C_{Ac} & C_{As} to get



C_{Ac} --(9)

$\frac{r_c}{R})$

n (2)

$C_{As}-C_{Ac})$

$\frac{1}{r_c}-\frac{1}{R})$ -(10)

(3) are used

termediate

C_{Ac} & C_{As} to get

$$-\frac{dN_A}{dt} = \frac{C_{Ag}}{\left[\frac{1}{4\pi R^2 k_g}+\frac{(R-r_c)}{4\pi D_e R r_c}+\frac{1}{4\pi r_c^2 k_s}\right]} \quad --(11)$$

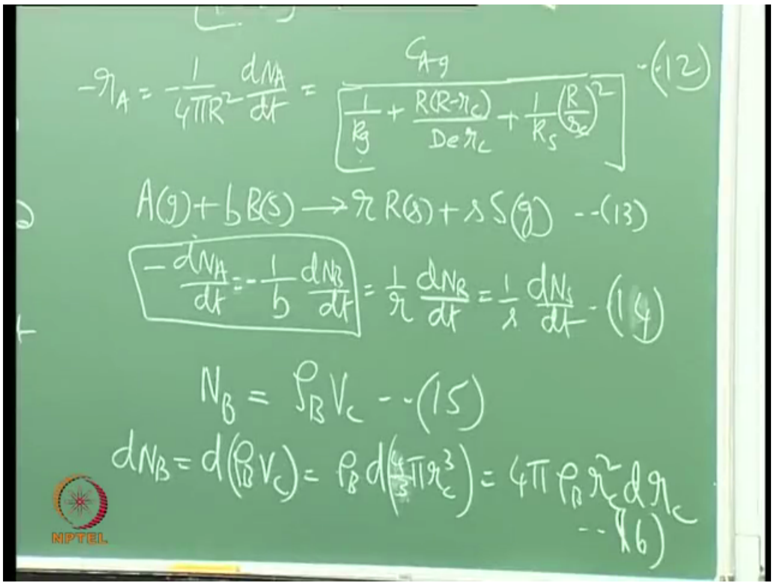
$$-r_A = -\frac{1}{4\pi R^2}\frac{dN_A}{dt} = \frac{C_{Ag}}{\left[\frac{1}{k_g}+\frac{R(R-r_c)}{D_e r_c}+\frac{1}{k_s}\left(\frac{R}{r_c}\right)^2\right]} \quad -(12)$$

$A(g) + bB(s) \longrightarrow r\,R(g) \quad (g)$ --(13)

$\boxed{-\frac{dN_A}{dt} = -\frac{1}{b}\frac{dN_B}{dt}} = \frac{1}{}\quad \frac{dN_s}{dt}$ -(14)

$N_B =$

$dN_B = d($ dr_c



$$-r_A = -\frac{1}{4\pi R^2}\frac{dN_A}{dt} = \frac{C_{Ag}}{\left[\frac{1}{k_g}+\frac{R(R-r_c)}{D_e r_c}+\frac{1}{k_s}\left(\frac{R}{r_c}\right)^2\right]} \quad -(12)$$

$$A(g) + bB(s) \longrightarrow r\,R(g) + s\,S(g) \quad --(13)$$

$$\boxed{-\frac{dN_A}{dt} = -\frac{1}{b}\frac{dN_B}{dt}} = \frac{1}{r}\frac{dN_R}{dt} = \frac{1}{s}\frac{dN_S}{dt} \quad -(14)$$

$$N_B = \rho_B V_c \quad --(15)$$

$$dN_B = d(\rho_B V_c) = \rho_B\, d\left(\frac{4}{3}\pi r_c^3\right) = 4\pi \rho_B r_c^2\, dr_c \quad --(16)$$

So that equation is dC A by dr at r equal to r c is C As C Ac divided by r c 1 minus r c by R this is equation number 9. Now I have equation 9 we can substitute here equation 2 then you know this is C As C Ac I can now eliminate intermediate concentrations, right. So I can also write this substituting equation 9 substituting equation 9 in 2 what you get is minus dN A by dt equal to 4 pi De ya okay C As C Ac divided by 1 by r c minus 1 by R that is the one so this is equation 10 so now the equations what I have 1 by r c minus 1 by R which is correct only you can just check ya so this is right, okay.

So now the equations what we have to solve is equations 1 and 10 and 3, right. So if I write that equation here then I will have 4 pi De and C As minus C Ac that is the one divided by 1 by r c minus 1 by R that is the equation. So we have to now eliminate concentrations of concentrations C Ac C As and express in terms of C Ag, right this again I will leave it to you at mathematical exercise how do you eliminate that, eliminate there are very simple techniques and also very complicated techniques, right so in the examination do not blame me you are supposed to know that.

So equation ya using equation 1, 10, 3 are used to eliminate intermediate concentrations intermediate concentrations C Ac and C As, good to get the equation that equation I will write here I think it may be (())(27:28) may not be sufficient here, to get minus dN A by dt equal to C Ag whole thing divided by 1 by 4 pi R square k g plus R minus r c divided by 4 pi De R r c plus 1 by 4 pi r square k s this is the equation, so this is equation number 11 but still this is not you know in useful form in the sense that it is extensive equation or intensive equation? By the way what is the difference between extensive and intensive? (())(28:41) as if you know if you do not know, Rinita you were telling something, depends on the mass.

How do you express the rate of reaction for homogeneous reactions definition of rate I am asking ya is it intensive or if I only express as dN A by dt is it intensive extensive or intensive know ya.

Student is answering: Intensive.

That means dN A by dt depends on if I take a large size particle or small size particle or if you take 10 mm particle, I take 1 mm particle, (())(29:34) may take 5 mm particle all three will get different rate but how do we normalize that so that we should talk the same language? By taking some ya either volume, mass or whatever per mass or volume, okay. So that is why here what is the logical one? Area.

So we can also express this as minus r A equal to minus 1 by 4 pi R square ya dN A by dt equal to after cancelling and all that C Ag 1 by k g plus R R minus r c by De r c plus 1 by k s into R by r c whole square r c whole square so this is the equation what we have for based on A, we have not talked anything till now about B but we would like to find out when the B is disappearing or when the disappearing in the sense that when the reaction is going to complete for B, right this is not directly useful for me because this gives me only the rate of reaction of gaseous space if you remember our stoichiometric equation.

But we are also interested this is useful if I am only worried about how the reaction you know gas phase reaction is taking place provided this r c at this particular r c at that point of time we can calculate what is the rate of reaction with respect to A we can calculate, right. But I also would like to find out how this r c is shrinking and when finally I will get 100 percent conversion? Or at any time what is the relationship between this r c that core and then the time this will not give me obviously you know that information so that is the next one using this information now you have to relate these two phases, right.

So when we relate that phases now we have to use the basic material balance that material balance is coming from this stoichiometric equation b B s giving me r R solid plus s S gas what is the relationship minus dN A by dt equal to 1 by b minus 1 by b dN B by dt equal to 1 by r dN R by dt 1 by s dN S by dt this is equation number 13, okay I think if I say this one as equation number 13 then this will be 14, okay so that is the relationship now, good.

So now again ya I can take these two and then relate dN A by dt I know already and if I that is nothing but 1 by b dN B by dt but still this is not useful to me because this N B is not giving me much information. So this I have to write in terms of r c in terms of r c, right our ultimate aim is to finally express this r c in terms of time okay ya correspondingly what is time and what is r c, r c gives me an idea about my conversion if r c equal to 0 conversion equal to 100 percent, if r c equal to capital R 0 conversion so in between that differentiation also we will make for X B, okay good.

So that is why we take this this relationship and we have N B, what is N B by the way? Kavya? Excellent number of moles of B how do I find out number of moles of B how do I find out number of moles of B? I have the particle and in this particle there are moles definitely how do we find out N B? Ya if we know that we have molar density and also mass density, if I know molar mass density then I have to divide by molecular weight and if I know molar density that is rho B we call rho B is the molar density this is rho B into V c, c is the volume of core, okay.

So ofcourse this V c equal to V volume of the particle at beginning then it slowly shrinks because we are only now trying to find out how the number of moles are getting slowly reacted, right okay. So now this equation please remember only one thing you have to important thing remember is rho B is not mass density rho B is moles per unit volume that you have to write make a note of that somewhere, okay.

So now dN B is differential of I am writing very very small steps also rho B V c is the rho B is constant when the reaction is taking place rho B is it constant, rho B it is the intrinsic property or extensive property, rho B per unit volume I said ya will it change it is same so that is why it is constant we will take it out, okay. So this is rho B d of V c which is nothing but 4 third 4 third pi r c cube ya correct no correct, Kayva still doubts, rho B okay you have taken let us say molar density let us say 10, okay right that is moles per unit volume, okay does that matter when you have this size, this size, this size does this matter or not assuming it is constant I think it is constant it will not change during the reaction if something happens it may change that is not I think you know that things we are not taking into account, right.

So the number of moles per unit volume of B is constant whether I may 1 centimetre cubic particle or 10 centimetre cubic or 100 centimetre cubic it is constant, it is constant still not able to get? Ya so that is why it is constant throughout you know please do not think that you know it is like normally with reaction concentration should change, concentration will change if you have everywhere you know for porous particle it changes, this is a non-porous particle very clearly we can identify this is the B may be logical doubt what she has.

If it is a porous particle B then I do not know where the how much B is available where inside the particle ya (())(38:17) ya A is gas ya for gas ya that is what the profile no and at r equal to r c at r equal to r c, okay whatever r c that comes there that will react with B but this molar density is constant because moles available in that unit volume is constant throughout, okay. So this is nothing but ya 4 pi r square 4 pi rho B r c square d r c ya so this is equation number 16, okay good.

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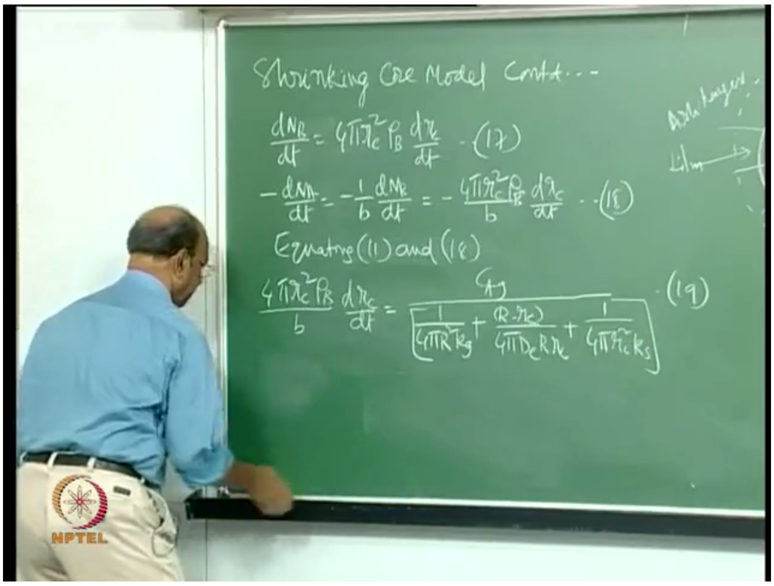


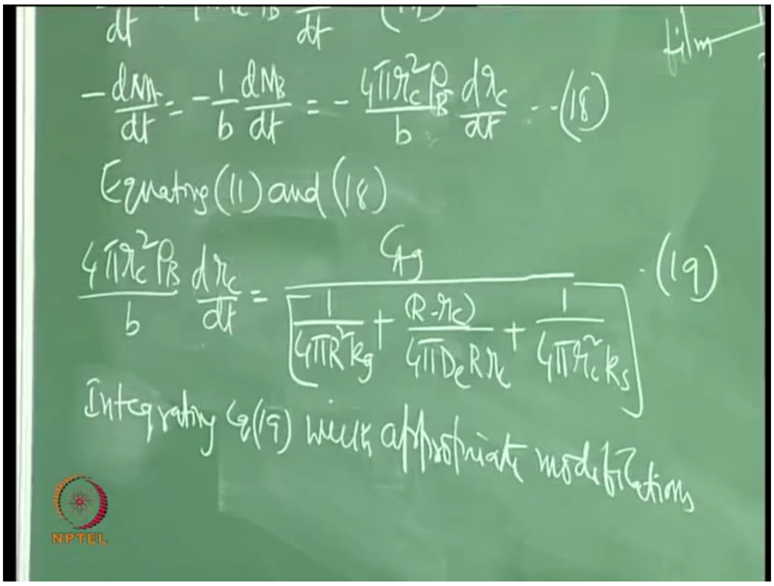
Shrinking Core Model Contd...

$$\frac{dN_B}{dt} = 4\pi r_c^2 \rho_B \frac{dr_c}{dt} \quad \text{...(17)}$$

$$-\frac{dN_A}{dt} = -\frac{1}{b}\frac{dN_B}{dt} = -\frac{4\pi r_c^2 \rho_B}{b}\frac{dr_c}{dt} \quad \text{...(18)}$$

Equating (11) and (18)

$$\frac{4\pi r_c^2 \rho_B}{b}\frac{dr_c}{dt} = \frac{C_{Ag}}{\left[\frac{1}{4\pi R^2 k_g} + \frac{(R-r_c)}{4\pi D_e R r_c} + \frac{1}{4\pi r_c^2 k_s}\right]} \quad \text{...(19)}$$



$$-\frac{dN_A}{dt} = -\frac{1}{b}\frac{dN_B}{dt} = -\frac{4\pi r_c^2 \rho_B}{b}\frac{dr_c}{dt} \quad \text{...(18)}$$

Equating (11) and (18)

$$\frac{4\pi r_c^2 \rho_B}{b}\frac{dr_c}{dt} = \frac{C_{Ag}}{\left[\frac{1}{4\pi R^2 k_g} + \frac{(R-r_c)}{4\pi D_e R r_c} + \frac{1}{4\pi r_c^2 k_s}\right]} \quad \text{...(19)}$$

Integrating Eq(19) with appropriate modifications

So now we will go to this side again okay what is that next thing we have to do dN by dt you can calculate dN by dt equal to we have 4 pi rho B r square d r c by dt, right. So 4 pi so this is equation 17 correct 17 ya that is right. So now we have the relationship minus dN A by dt equal to minus 1 by b dN B by dt equal to minus 4 pi r c square rho B by b small b, b is the stoichiometric coefficient d r c by dt this is equation 18.

Now we have some relationship between 18 and then that equation 12, right this one or this one equation 11 minus dN A by dt. So now I will equate 11 and 18 with appropriate multiplications, right ofcourse here I have minus 1 by b dN A by dt I do not have to multiply anything. So now equating 11 and 18, now I have the relationship between r c I have the relationship between r c ya so we have to integrate after separating the variables because now this one, okay let me write this step 4 pi r c square rho B by b ya d r c by dt equal to I have here C Ag 1 by whole thing divided by 4 pi r square ya plus capital R minus r c divided by 4 pi De R r c plus I have another term 1 by 4 pi r c square k s is the one, these two we have equated.

Now you know r c and this contains r c so I can bring this side and other constant terms I can bring that side so dt will come this side, d r c will be here then we can integrate and after integration that also I do not give integration I will give after integration and rearranging right this is equation number 19, okay ya integrating equation 9 with appropriate arrangements integrating appropriate modifications, okay.

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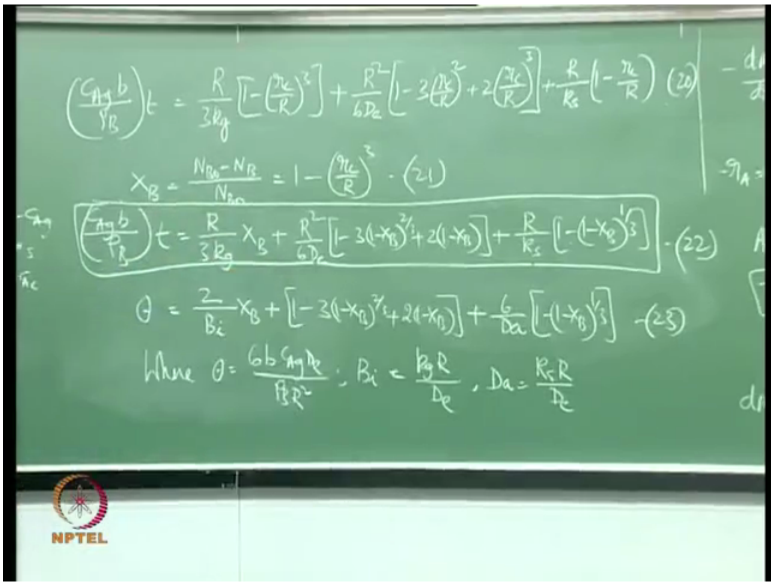


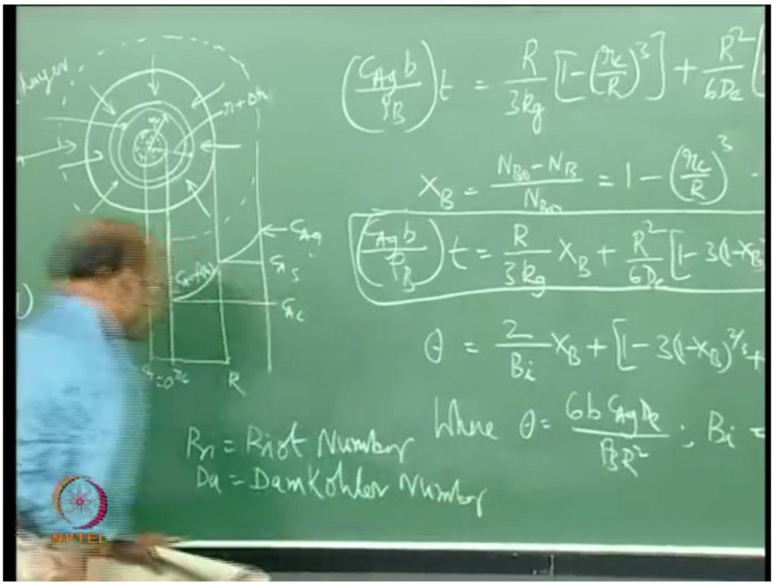
$$\left(\frac{C_{Ag}\,b}{\rho_B}\right)t = \frac{R}{3k_g}\left[1-\left(\frac{r_c}{R}\right)^3\right] + \frac{R^2}{6D_e}\left[1-3\left(\frac{r_c}{R}\right)^2+2\left(\frac{r_c}{R}\right)^3\right] + \frac{R}{k_s}\left(1-\frac{r_c}{R}\right) \quad (20)$$

$$X_B = \frac{N_{B0}-N_B}{N_{B0}} = 1-\left(\frac{r_c}{R}\right)^3 \quad (21)$$

$$\boxed{\left(\frac{C_{Ag}\,b}{\rho_B}\right)t = \frac{R}{3k_g}X_B + \frac{R^2}{6D_e}\left[1-3(1-X_B)^{2/3}+2(1-X_B)\right] + \frac{R}{k_s}\left[1-(1-X_B)^{1/3}\right]} \quad (22)$$

$$\theta = \frac{2}{B_i}X_B + \left[1-3(1-X_B)^{2/3}+2(1-X_B)\right] + \frac{6}{Da}\left[1-(1-X_B)^{1/3}\right] \quad (23)$$

Where $\theta = \frac{6b\,C_{Ag}D_e}{\rho_B R^2}$; $B_i = \frac{k_g R}{D_e}$, $Da = \frac{k_s R}{D_e}$



Bi = Biot Number
Da = Damkohler Number

What you get is this equation that is may not be sufficient here ya what you get is C Ag b by rho B into t equal to R by 3 k g plus R square 6 De 1 minus 3 1 minus 3 r c by R whole square whole cube ya plus R by k s 1 minus r c by capital R this is equation number 20 ya this is the equation this is the one. So now I have a relationship between r c and then the t but all this mathematics you have to do do not blame me when I give this in the examination atleast you have to do that, okay very simple you know high school integration, it is not at all great difficult integration.

So now this also as engineers particularly chemical engineers we are interested happily in terms of conversions, so how do I find out this equation in terms of conversions, okay how do we define conversion? Conversion x equal to initially what are the moles minus moles left divided by initial moles, even here when I have X B we are now interested r have come into in terms of X B, okay so X B equals to N B not minus N B by N B not, please give me the equation no in terms of r c that is the one just try it and then tell me, in terms of r c 1 minus excellent, 1 minus r c by that is the equation, okay.

So now I have r c by R cube, r c by R square r c by R square so this is r c by R so then correspondingly I can write this equation in terms of this is equation 21 so writing the equation 20 in terms of conversions what you get is C Ag b rho B into t equal to R by 3 k g ya this one will be X B plus R square by 6 De 1 minus 3 1 minus X B 2 by 3 plus 2 1 minus X B ya that is all plus we have R k s 1 minus 1 minus X B to the power of 1 by 3 ya so this is the expression which gives me the relation between conversion and time.

So you can now calculate when X B if you want 100 percent you know X B equal to 1, you can substitute there and then it will be in terms of k g, De, k s and capital R okay this is beautiful this one I have solved this equation using all three resistances same time but if you see Levenspiel which you would have studied definitely and you would have forget it totally and you know if you see that every step we take separately diffusion you know first mass transfer of A through film controlling, then diffusion controlling, then reaction controlling. The same thing even now we can do that here, okay after taking the general expression like for example if k s is very very large which is controlling? Reaction is controlling, mass transfer which mass transfer is controlling? There are two one is diffusion, other one is ya convection through the film.

So that is why every time now we can take ofcourse individual steps controlling means if it is mass transfer control this k g, De is very large, k s is very large. So like that that simplifications we will discuss in the next class ya and ya just before that one more thing this equation can also be written in terms of dimension less quantities which is very important for chemical engineers dimension less.

So how we write this equation only one equation I just write is something like this write this in terms of dimension less. So this is theta time equal to 2 Biot number into X B plus I have 1 3 1 minus X B to the power of 2 by 3 plus 2 1 minus X B plus I have 6 by Da 1 minus 1 minus X B of 1 by 3 this is equation number 23, where theta equal to 6b C Ag De divided by rho B R square that is the definition of theta that is 1 and Biot number biot number Bi ya anyone knows about this Biot number? k g R by De, Bi is Biot number Biot and Da is Damkohler number which is k s R by De, okay.

So I think I can also write here Bi equal to Biot number and Da equal to Damkohler number ya Damkohler number, right I think next class we will discuss the significance of this the meaning of Biot number very large for example which should be controlling and most of the time in gas solid reactions you first calculate Biot number and then if it is very large you neglect film step that means neglect in the sense that film is not controlling.

That means Biot number large means k g must be very large and diffusion must be very small, diffusion very small means diffusion controlling, k g is anyway very large for large Biot numbers. So that is why one has to get this kind of estimations in the beginning which one is rate controlling step, Damkohler number means it is reaction and diffusion, right if Damkohler number is small that means De should be very large and k s should be small that means it is reaction control.

So that is why you have these numbers which will give you some physics to understand, okay I think we will stop here tomorrow we will discuss about the individual steps controlling and how do you find out the diffusivity, how do you find out k g, how do you find out k s all that is important otherwise we do not know how to use that equation, equation 22 and 23 are beautiful equations, okay for gas solid reactions non-catalytic, okay thank you.