Advanced Chemical Reaction Engineering
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Lecture - 28
Shrinking Core Gas Solid Reactions Model

We will look at gas solid reactions today.

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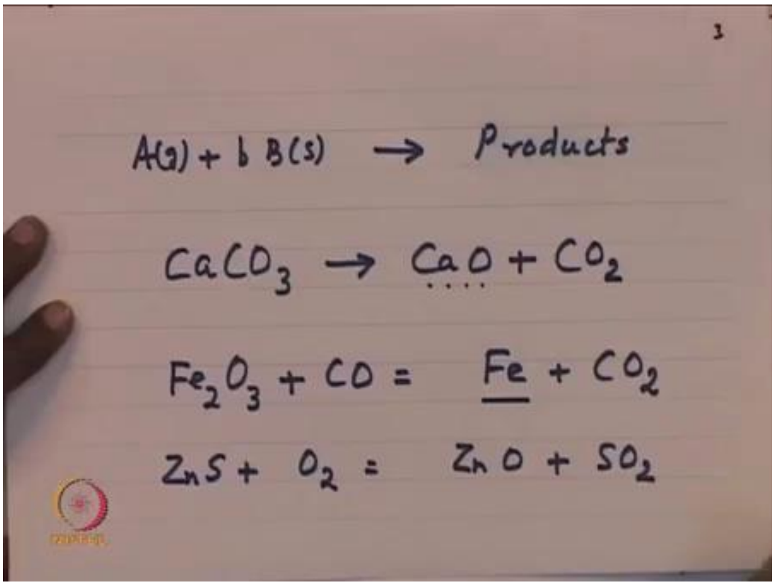

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$$A(g) + b\,B(s) \rightarrow \text{Products}$$

$$CaCO_3 \rightarrow \underline{CaO} + CO_2$$

$$Fe_2O_3 + CO = \underline{Fe} + CO_2$$

$$ZnS + O_2 = ZnO + SO_2$$

Now there are several examples of interest to us, in which we want to react say a gas with a solid which gives us products. Now we can look at several types of examples, simple example would be let us say we have calcium carbonate and it under goes decomposition. It gives us calcium oxide plus carbon dioxide or a very common example would be an oxide reacting with carbon monoxide, giving you iron plus c o 2. We can balance this reaction, now whenever we looking at a gas solid reaction of course our prime interest is to see that the product we get is of good quality.

We want the product is of good quality, in other words we do not want un reacted material in the product. Let us take one more example, zinc sulfide plus oxygen giving you zinc oxide plus sulfur dioxide. Now, these are all commercially extremely important reactions, millions of tons of products are produced by these reactions. Each of them great value to us in daily life they, if we look at reactions like zinc sulfide, zinc is a available in this form called zinc blend, reacts with oxygen to form zinc oxide in sulfur dioxide.

Notice here this sulfur dioxide is also very valuable product, on other words is this zinc sulfide does not react completely then, part of the sulfur is also lost. Because, sulfur dioxide is use for making sulfuric acid. Therefore, in sharing the this reaction actually goes to completion is of great interest to us. Therefore, in whatever we do we would like to understand how to manage the reactions so that, variable to drive the reaction to completion. Let us look at some simple examples to understand what might be the way to handle all this.

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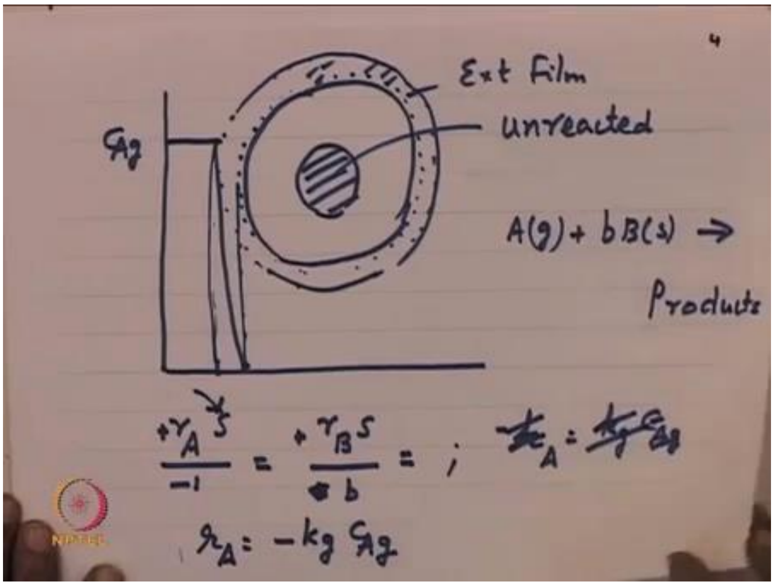

$$\frac{+r_A^{s}}{-1} = \frac{+r_B^{s}}{b} = \; ; \quad \cancel{-r_A} = \cancel{k_g C_{Ag}}$$

$$r_A = -k_g C_{Ag}$$

So, let us say you have a circle solid. Now let us say that this solid was of this size, where we started and due to reaction it has become of a smaller size. On other words the material which is unreacted this is unreacted this is unreacted. So, when we started the whole thing was unreacted, now as a reaction proceeded part of it is gotten to reacted. We want to understand, we want to understand how this whole things was reaction proceeds. We will take, once again we will just raking nice a gas plus b B solid giving you products. Let us for a moment assume that, the film which is on the outside of this solid, there is a gas film which is in the outside of the solid, on the solid. And all the resistance to supply of the gas is in this external film.

So, on other words you have I mean, I am just draw this external film in a slightly big way so, I mean this is, I mean, it is, I am just drawing it slightly big so that, you know we understand that you know it is, this is the external film. I will call this as the external film, external film. So, this gas concentration let us say, gas is coming so this is the gas, gas is here and in this distance they concentration of gas becomes 0. So, if you start at c A g is a concentration of gas and as it enters the film, it concentration drops from c A g to 0. On other words, the rated which this supply of gas to the solid surface is controlled by the resistance in the external film.

So, we know from our basic and the standing that as the velocity of gas all the solid changes, this external film thickness changes. In fact decreases velocity increases, to an extent we can control this rate of transfer by managing the velocity of gas over the solid. So, if this is the reaction then we can say A if based on our understanding stoichiometry by minus of 1, sorry equal to r B s divided by minus b sorry, minus b that is equal to this is, these two are equal because is the fact that it is stoichiometry. And also we say that r A with a minus sign is k g times c A g. How do we understand this that, the rated which this is r, this is not written properly. This is rate r a, this is rate of supply, the rated which chemical reaction takes place.

What we saying is that we have a circle part now, the rated which the gas is supplied to the solid surface is controlled by external diffusion, that is the case we considering right now. Therefore, we have the rate at which can be reaction occurs is minus of k g times c A g k g is a ((Refer time: 06:36)) coefficient, c A g is the gas concentration. We assuming that the gas outside is in large quantity therefore, as a reaction proceeds the change in the concentration of gas external to, on the outside as solid does not, is not significant. And therefore, we can ignore it at least for the movement in this formulation. Now we know from stoichiometry that r A times s by minus 1 is r B times s by minus b.

So, this basically statement of stoichiometry the word, this term s refers to the surface area of solid, which is in responsible for reaction. On other words for it trained say here that, in gas solid reaction surface area is very important. Therefore, r A is reaction rate for unit area if you multiplied by s details you the total reaction rate. Now if you want to find out what happens to the solid after all our interest is to find out what happens to the solid and how the solid changes.

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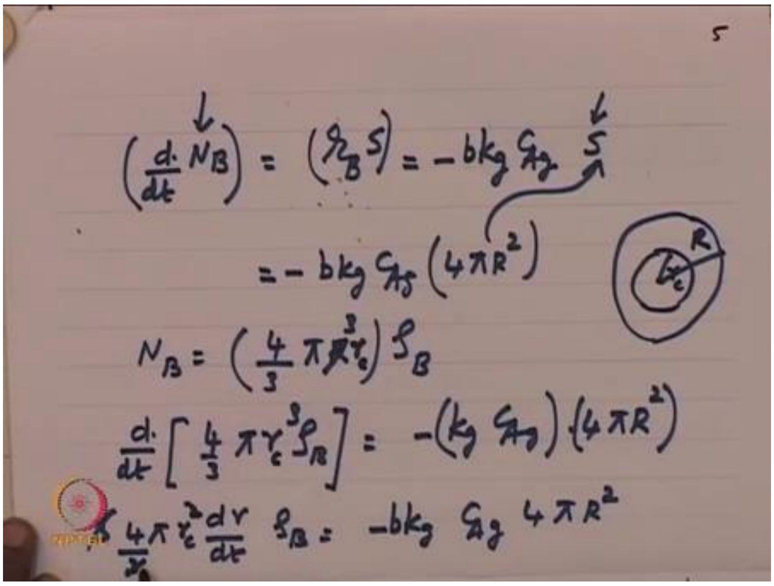

$$\left(\frac{d}{dt} N_B\right) = (r_B s) = -b k_g C_{Ag} s$$

$$= -b k_g C_{As} (4\pi R^2)$$

$$N_B = \left(\frac{4}{3}\pi r_c^3\right) \rho_B$$

$$\frac{d}{dt}\left[\frac{4}{3}\pi r_c^3 \rho_B\right] = -(k_g C_{Ag})(4\pi R^2)$$

$$\frac{4\pi}{3} 3 r_c^2 \frac{dr}{dt} \rho_B = -b k_g C_{Ag} 4\pi R^2$$

So, we write here our material balanced by d t of N B, this is the rated which change it must be equal to r B times s. We understand this, d by d t is r B times s. So, what is r B times s we have said this minus of k g times A g times s.

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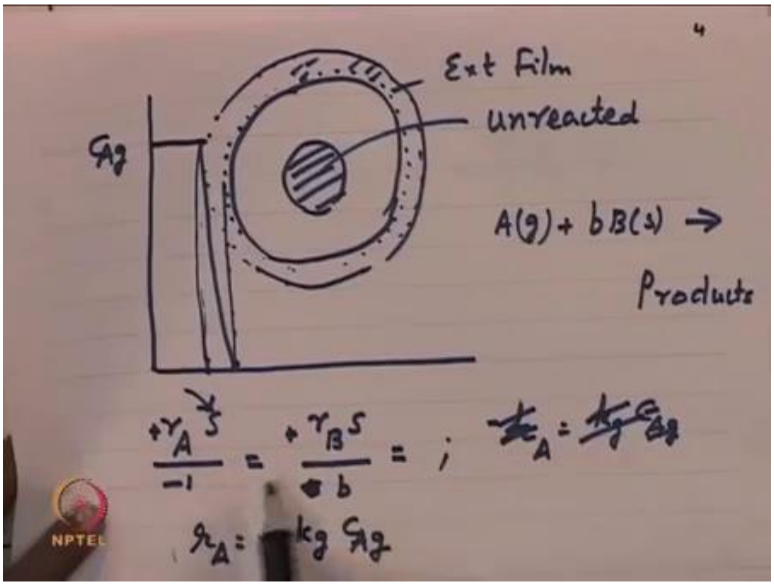

$A(g) + bB(s) \rightarrow$ Products

$$\frac{+r_A s}{-1} = \frac{+r_B s}{-b} = ; \quad \cancel{-r_A = k_g C_{Ag}}$$

$$r_A = -k_g C_{Ag}$$

Please recognize here so, r B times s is the rate of chemical reaction. Now, what is r B times s is related to r A times s, we have to multiply by this stoichiometry is that clear, what we are saying? Therefore the rate at which the solid changes, that means the rate number of molds in N B, the rate at which changes is equal to r B times s, which is minus of b times k g times c A g multiplied by s, which is a surface area which is appropriate to the controlling regime. What is the surface area through which the supply of gas is contacts solid? Whatever may be this state of the unreacted core, we find that the surface area through which that oxygen, the material has to defuse is the external surface area, which is sizes of the radius, if it is r the external surface area is 4 pi r square.

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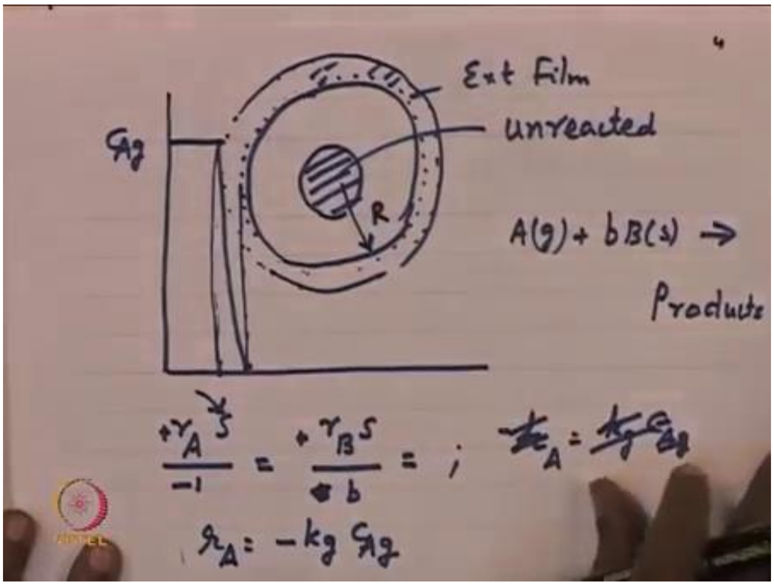

$$\frac{+r_A \cancel{S}}{-1} = \frac{+r_B S}{-b} = \; ; \quad \cancel{-r_A} = \cancel{k_g C_{Ag}}$$

$$r_A = -k_g C_{Ag}$$

Therefore, surface area s that is relevant for this controlling regime is c A g times 4 pi r square. Let us go through this formulation once again, what we have saying we having a spherical particle of radius r, this spherical particle radius r is in contact with the large quantity of gas and it undergoes chemical reaction.

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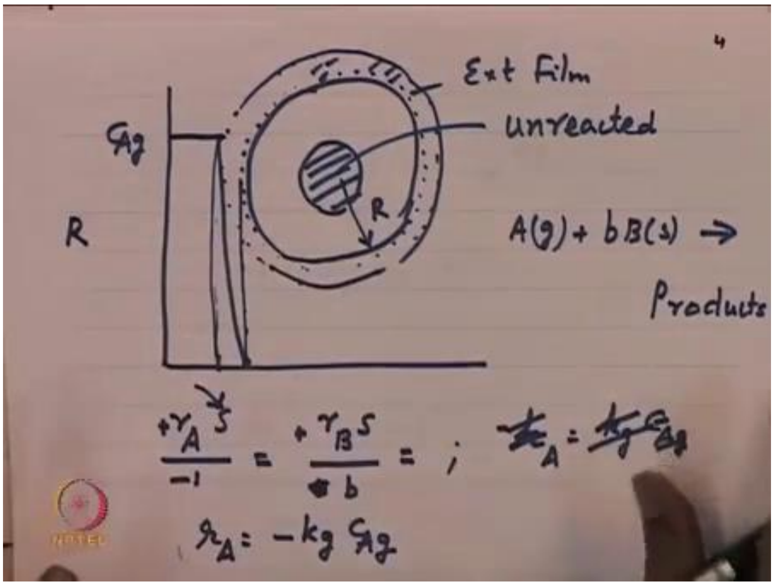

And this chemical reaction is controlled by rate at which the gas is supplied to the solid surface and that rate of supply of gas is taken as k g times c A g with a minus sign showing that component a is getting consumed because of the reaction. Now the surface area which is relevant to this supply is the external surface area because, that external surface area is 4 pi r square. Therefore, we have on the basis of these that the rate at which the solid b changes is r B times s, which is minus of b time k g time c A g time s. Where, this surface area refers to the external surface area and what is N B by definition? N B by definition is the unreacted material, whose quantity is this multiplied by density refers to total number of ((Refer Time: 10:18)).

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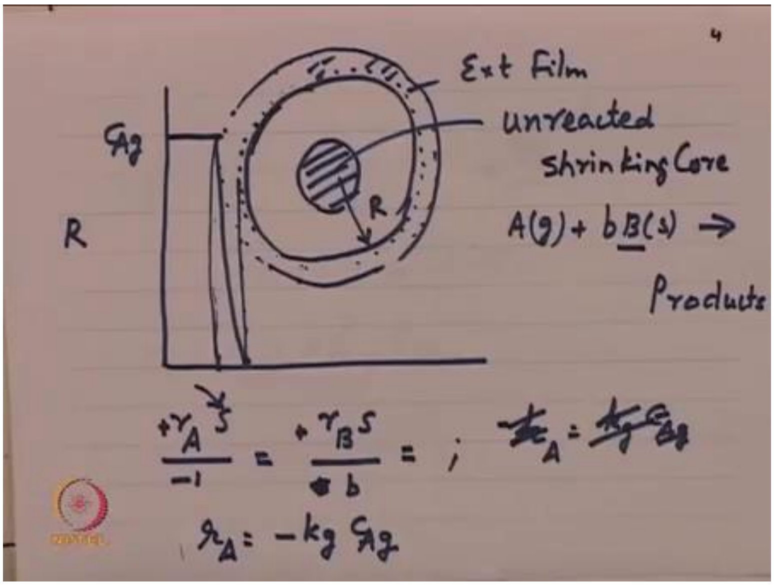

$\frac{+r_A^{s}}{-1} = \frac{+r_B^{s}}{b} = \; ;$ ~~$-r_A = k_g C_{Ag}$~~

$r_A = -k_g C_{Ag}$

So, what is our model? Our model is we look upon the solid which is undergoing chemical reactions as that of a sphere, which undergoes chemical reaction. And as the reaction proceeds, as a reaction proceeds the unreacted material which is initially here, it keeps on progressing inwards or unreacted cores keeps on shrinking. Therefore, it is also called as a shrinking core model. So, what is our model we have a solid spherical particle, which is in contact with the gas of concentration c A g and this concentration does not change.

Because, the amount of gas is so large that the change in the gas concentrations are taken as unimportant in this formulation, we will relax all this in the go long. Now, as a reaction proceeds the unreacted surface which is initially of radius r, this unreacts surface keeps on shrinking as a reaction proceeds. So, this is the reacted material is this, this is reacted material, this is the unreacted material. So, our interest is to find out how the radius of the unreacted core, this is the radius that the initially it is r. Now the radius is let us say small r, unreacted core, how the radius is the unreacted core changes as a reaction proceeds.

This is what, so this equation here now that we know we can substitute for N B we get d by d t of 4 by 3 pi, this is at any time which is small r so, pi r cubed times rho B. So, this is left hand side you could have minus of k g c A g and now we know that the area this, that is relevant to this supply of the reagents, that is 4 pi r squared. Even if the core radius keeps on shrinking, even if the unreacted core which keeps on shrinking, the surface area of through which is supply of reaction takes place that is 4 pi capital R squared, that surface area does not change. Even though the reaction, the core which is unreacted keeps on shrinking.

So, what do we get? We get that d r d t 3 cancels of so, we get 4 pi, 4 pi r d t row b equal to minus of k g c A g 4 pi r squared just check we got everything, right? So, here we get 4 pi r d r c by d t so, when we differentiate this, it becomes r c squared there is a 3 here, there is a 3 here, which cancels of r c squared here, have you got it right, rho B 4 pi r c square d r c by d t minus of b missing here, b is here, b k g c A g 4 pi capital R square. This tells you how the general approach here is to call this is r c, to indicate that the core, this is the unreacted core, this is the unreacted core and initially the radius of the unreacted core was capital R.

So, the capital R is the radius of the particle which, but r c is the radius in the unreacted core which is shrinking, because of the chemical reaction. So, we have setup the equations properly here, N B 4 by r c cubed, times rho B. So, I put all the numbers here so that the equation looks like this.

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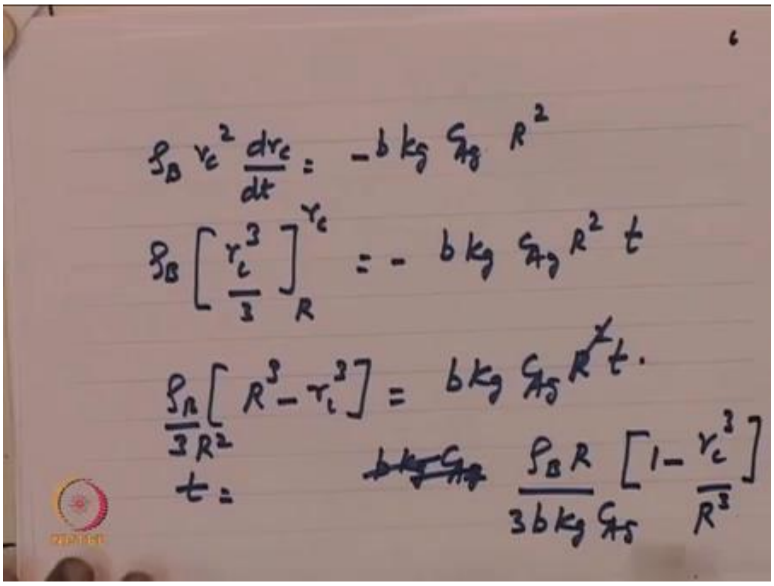

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$$\rho_B r_c^2 \frac{dr_c}{dt} = -b k_g C_{Ag} R^2$$

$$\rho_B \left[\frac{r_c^3}{3}\right]_R^{r_c} = -b k_g C_{Ag} R^2 t$$

$$\frac{\rho_B}{3R^2}\left[R^3 - r_c^3\right] = b k_g C_{Ag} R^{\cancel{2}} t.$$

$$t = \cancel{b k_g C_{Ag}} \frac{\rho_B R}{3 b k_g C_{Ag}}\left[1 - \frac{r_c^3}{R^3}\right]$$

So, let me simplify this a little r c square d r c by d t equal to minus of k g c A g r squared because, you cancel the 4 pi. Now we can integrate this so that, the integrate form becomes r B divided by, when I integrate this becomes r c cube by 3, it goes from we started R and goes to r c equal to minus of b k g c A g, b is missing here R squared and time. Now put the limits it becomes b times and take the minus sign on this side, it becomes R cubed minus r c cubed divided by 3 equal to b k g c A g R square t. Now I can divide throughout by r here so, I put R square here.

So, this whole thing can be written as t equal to b k g c A g, have you got it right? t equal to not like this, like this t equal to, t equal to rho B r divided by 3 b k g c A g with in brackets of 1 minus of r c cube by R cubed, have you got it right? That is equal to time. So, simply take r cube outside, it simplifies like this.

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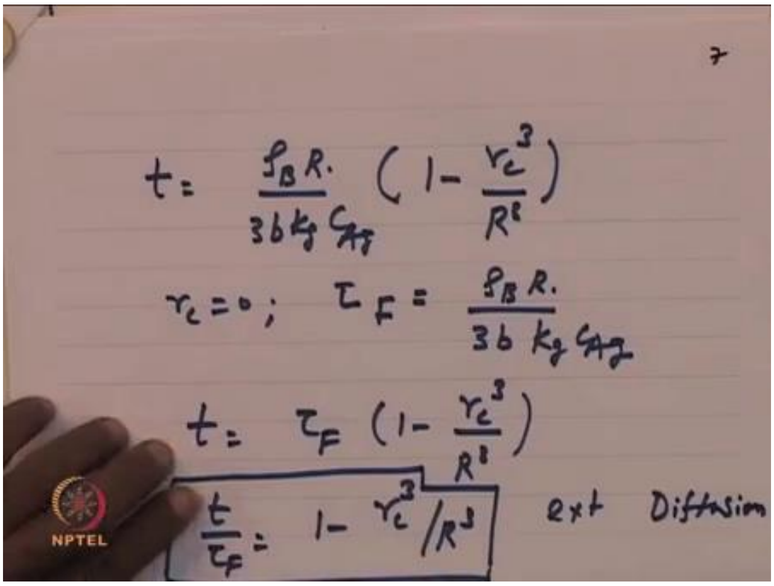

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$$t = \frac{\rho_B R.}{3 b k_g C_{Ag}} \left(1 - \frac{r_c^3}{R^3}\right)$$

$$r_c = 0 ; \quad \tau_F = \frac{\rho_B R.}{3 b \, k_g C_{Ag}}$$

$$t = \tau_F \left(1 - \frac{r_c^3}{R^3}\right)$$

$$\boxed{\frac{t}{\tau_F} = 1 - r_c^3 / R^3} \quad \text{ext Diffusion}$$

So, let me write it once again just to put it in a nice form. So, time required for complete, for reaction of this particle under what I call as external diffusion control is given by t equal to rho B R divided by 3 times b, which is a stoichiometry coefficient. k g is the ((Refer Time: 16:28)) coefficient and c A g is the bulk concentration which is assumed to be unchanging. Now what happened when r c becomes 0, which means the particle fully consume or I can call this as the time required for complete consumption of the particle, when the external film controls. So, what is tau f? Time require for complete consumption when external film diffusion controls, so that is equal to rho B R divided by 3 b k g times c A g.

So that, now what it becomes is that, time required is simply 1 minus r c cubed by R cubed or t divided by tau f is 1 minus of r c cubed by R cubed. So, this relationship tells us that if there is external diffusion which is controlling. Then, the time required for complete consumption particle or timed required for consumption of a certain mode particle is given by 1 minus r c cube by R cubed.

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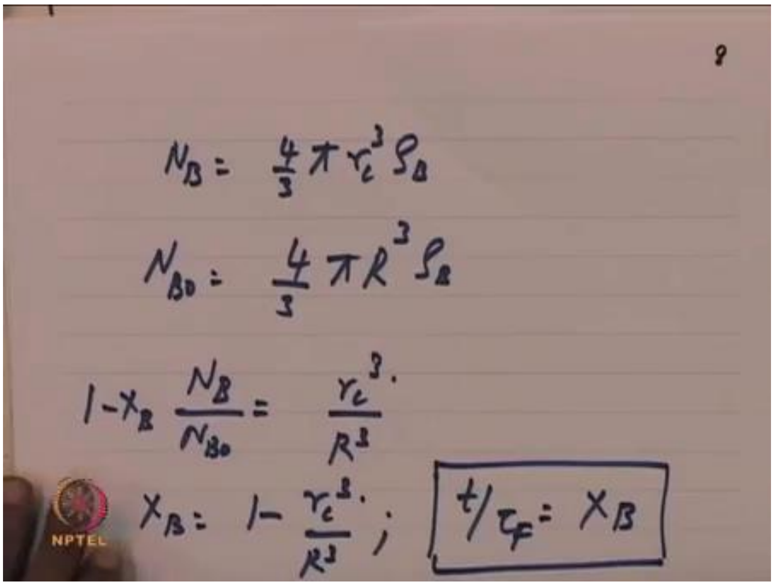

$$N_B = \frac{4}{3}\pi r_c^3 \rho_B$$

$$N_{B0} = \frac{4}{3}\pi R^3 \rho_B$$

$$1 - X_B \quad \frac{N_B}{N_{B0}} = \frac{r_c^3}{R^3}.$$

$$X_B = 1 - \frac{r_c^3}{R^3}. ; \quad \boxed{t/\tau_F = X_B}$$

Now we also know from our basic understanding is that N B which is a total particle that us present is 4 by 3 pi r c cube tan 0 b. And we also know N B is 0 equal to 4 by 3 pi R cubed times rho b. Therefore, what is this ratio N B divided by N B 0 by definition is 1 minus of X B which is a conversion of the solid, that ratio is equal to r c cubed by R cubed. On other words, we can also write this equation t by tau f which is 1 minus r c cubed R cubed we can sight here. Therefore X B equal to 1 minus of r c cubed by R cubed and therefore, we writes t by tau f is also equal to X B. This is a result which comes out of our understanding of the system.

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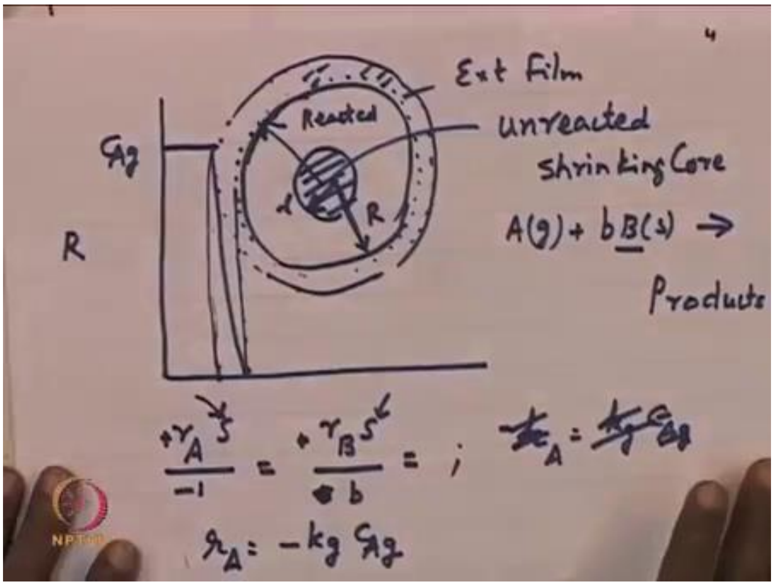

$$\frac{+r_A s}{-1} = \frac{+r_B s}{b} = \; ; \quad \cancel{-r_A = k_g C_{Ag}}$$

$$r_A = -k_g C_{Ag}$$

What are you saying now? What are we saying is if you have a spherical particle, which is undergoing chemical reaction, which is undergoing chemical reaction under external film diffusion control. If this solid is in contact with a large quantity of gas and this reaction takes place, as a result of this reaction the core keeps on shrinking, unreacted core keeps on shrinking.

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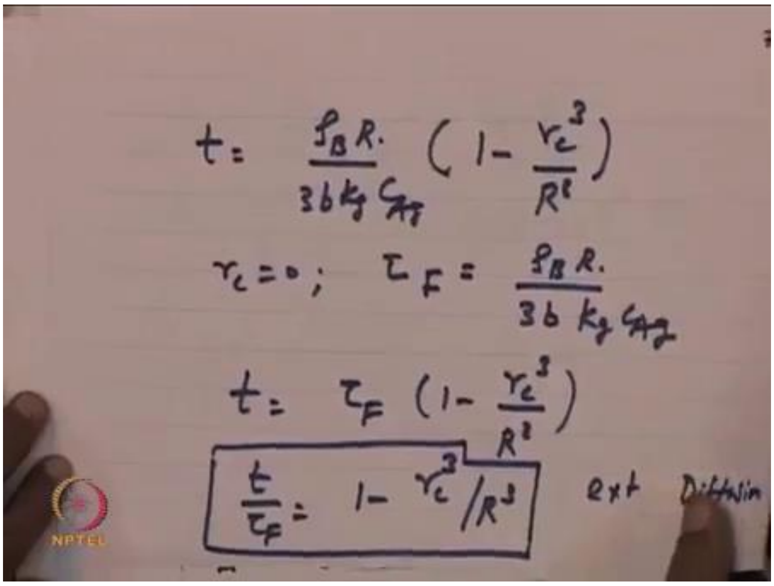

$$t = \frac{\rho_B R}{3b k_g C_{Ag}} \left(1 - \frac{r_c^3}{R^3}\right)$$

$$r_c = 0; \quad \tau_F = \frac{\rho_B R}{3b\, k_g C_{Ag}}$$

$$t = \tau_F \left(1 - \frac{r_c^3}{R^3}\right)$$

$$\boxed{\frac{t}{\tau_F} = 1 - r_c^3/R^3} \quad \text{ext Diffusion}$$

And then we have the our equations which says that, the time required for complete consumption to, the time require for any extent of reaction, time requires complete consumption is given by 1 minus r c cube R cubed. And when we recognize some of these simple relationships, we will notice that the extent of reaction X B is equal to t by tau f, that is how this relationship nicely comes.

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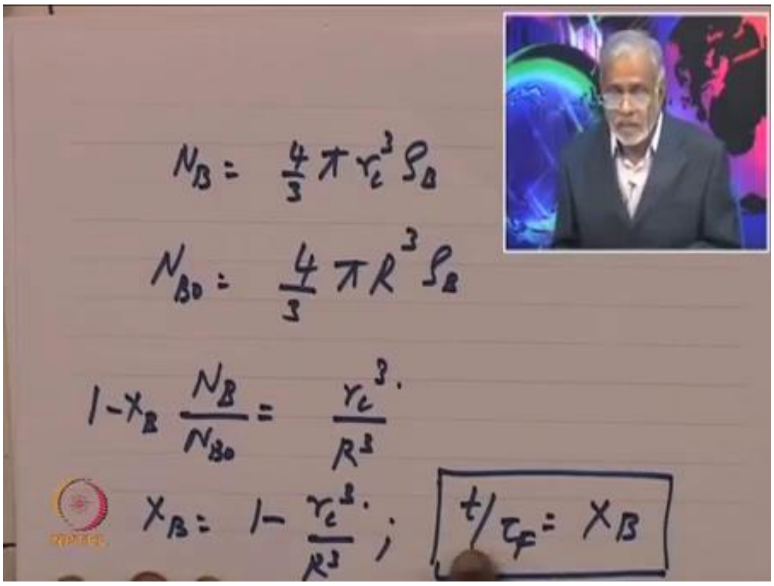

$$N_B = \frac{4}{3}\pi r_c^3 \rho_B$$

$$N_{B0} = \frac{4}{3}\pi R^3 \rho_B$$

$$1 - X_B \quad \frac{N_B}{N_{B0}} = \frac{r_c^3}{R^3}$$

$$X_B = 1 - \frac{r_c^3}{R^3} ; \quad \boxed{t/\tau_f = X_B}$$

So, for the case of external diffusion control we have the extend of reaction of X B is simply t divided by tau f. So, if you want to find out a case why there is external diffusion kind of control, similarly find the time required by complete consumption, time required at any given instant of time, that ratio is the extent with the reaction is occurred.

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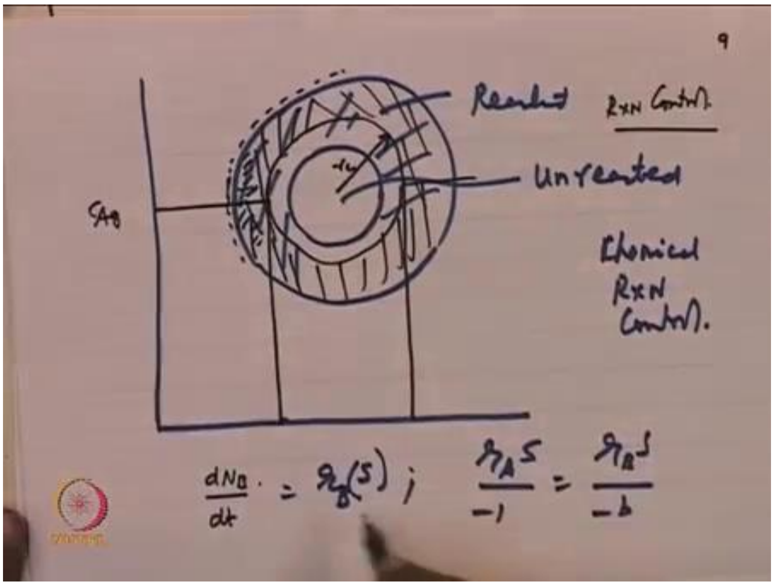

$$\frac{dN_B}{dt} = r_B(s) ; \quad \frac{r_A s}{-1} = \frac{r_B s}{-b}$$

Our next example is we have a particle, we have a shrinking particle, sorry we have a particle which undergoes reaction. So, what does it mean the particle is undergoing reaction means, we have this is the reacted core, this is reacted core, this is reacted. So this is unreacted, in this case we are looking at the case where, this reaction that is taking place is controlled by chemical reaction, chemical reaction control. What is meant by chemical reaction control is that, let us say at any instant of time, at any instant of time the, this is the what we call as the reacted core let us at instant of time, let say this the reacted core.

So what we are saying is, what we are saying is that, the concentration of the gas remains at c A g and as it reaches the solid surface it drops to 0. So, in the same way here concentration remains like this, it drops to 0. So, what we trying to say here is that there is no drop in concentration of gas as it moves through the external film. There is an external film here, we can see external film and as it moves through the reactant layer, this is reactant layer, this is called reacted layers you see. So, the assumption here is this reaction control, reaction control means what?

It means that all the resistance lies in the at the reaction surface therefore, there is no drop in concentration as it moves through external film, as it move through the reacted components and as it comes to a surface it drops to 0. When concentration at the surface drops to 0, when the concentration at the surface drop to 0 means it is a irreversible reaction. Now if the concentration does not drop 0, it means an it is a reversible reaction so that, the surface concentrations will be appropriately described by the equilibrium relationship. As of now we taking the surface concentration to going 0 therefore, it is an irreversible action.

So, for reaction control we have d N B by d t, d N B by d t as usual equal to r B times s. We also know r A s with the minus 1 equal to r B s with a minus b, this also we know because stoichiometry. Then what is s, what is s, which is appropriate to reaction control? We recognize that as a reaction proceeds, the surface area there is appropriate to the reaction is unreacted core surface. So, as a core keeps on shrinking the unreacted core of radius r c, it keeps on shrinking. Therefore, value of s refers to 4 pi r c squared. So, here s refers to 4 pi r c square.

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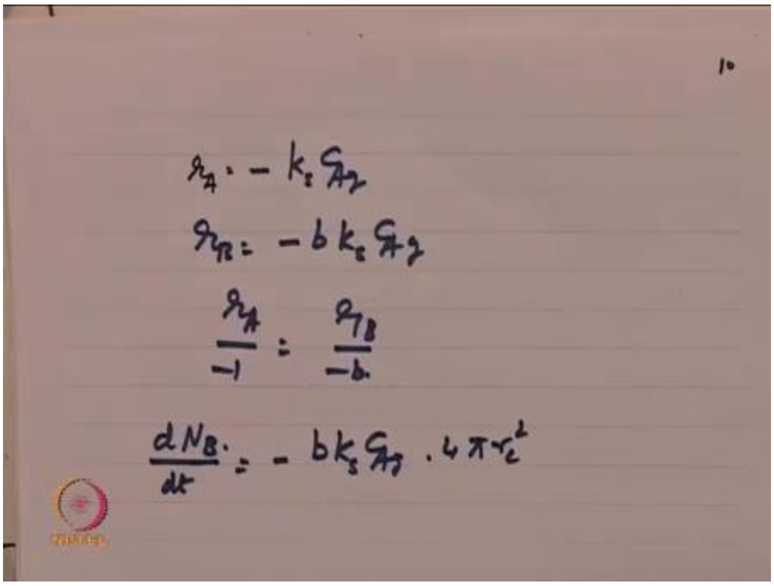

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$$r_A = -k_s C_{Ag}$$

$$r_B = -b k_s C_{Ag}$$

$$\frac{r_A}{-1} = \frac{r_B}{-b}$$

$$\frac{dN_B}{dt} = -b k_s C_{Ag} \cdot 4\pi r_c^2$$

So that now we can write, what is our rate functions we have r A, r A which is a rate of chemical reaction is equal to minus of k s time c A g, r B equal to minus of b times k times c A g, you see. And we also know r A times minus of 1 equal to r B times minus of b therefore, we get this relationship. So, what is d N B by d t so d N B by d t equal to minus, what is this relationship minus of b times k s time c A g multiplied by the area which is appropriate to the process. We said the area which is appropriate to reaction control, is the area which is unreacted surface and any instant of time the radius is the unreacted core is r c.

So, where that particular surface area is 4 pi r c square. So, this equation represents the variation of what is happening to component b, as a reaction proceeds.

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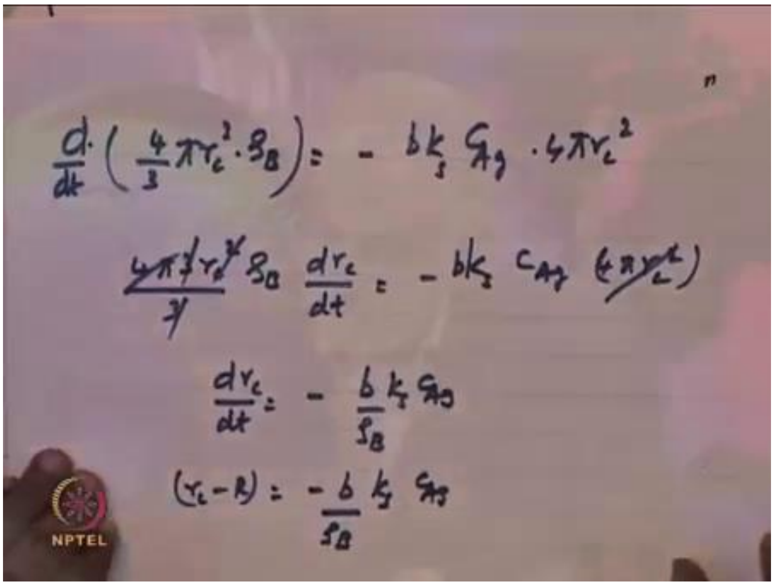

$$\frac{d}{dt}\left(\frac{4}{3}\pi r_c^3 \cdot \rho_B\right) = - b k_s C_{Ag} \cdot 4\pi r_c^2$$

$$\frac{4\pi \cancel{3} r_c^{\cancel{3}} \rho_B}{\cancel{3}} \frac{dr_c}{dt} = - b k_s C_{Ag} \left(\cancel{4\pi r_c^2}\right)$$

$$\frac{dr_c}{dt} = - \frac{b}{\rho_B} k_s C_{Ag}$$

$$(r_c - R) = - \frac{b}{\rho_B} k_s C_{Ag}$$

So, we get know here the left hand side if 4 by 3 pi r c cubed times rho B. So, this is the left hand side d by d t equal to what is our right hand side b times k s times c A g times 4 pi r c square. This refers to the surface area, which is relevant to the controlling surface area, this surface area was 4 pi capital R square when we talked about external film diffusion control. So, the surface area for reaction control is the unreacted core surface was a reaction is taking place, which is 4 pi r c squared. Let me simplify this so, 4 pi so, it is r c square into 3 divided by 3 rho B d r c by d t minus of k s c A g 4 pi r c squared. 3 cancels off 4 pi cancels off, cancels off.

So, we will get d r c by d t minus of b k s c A g by rho b, integrating this is r c minus of R equal to minus of b k s c A g by rho B. Or we can simplify this further, we can simplify this further and write this as, write this as.

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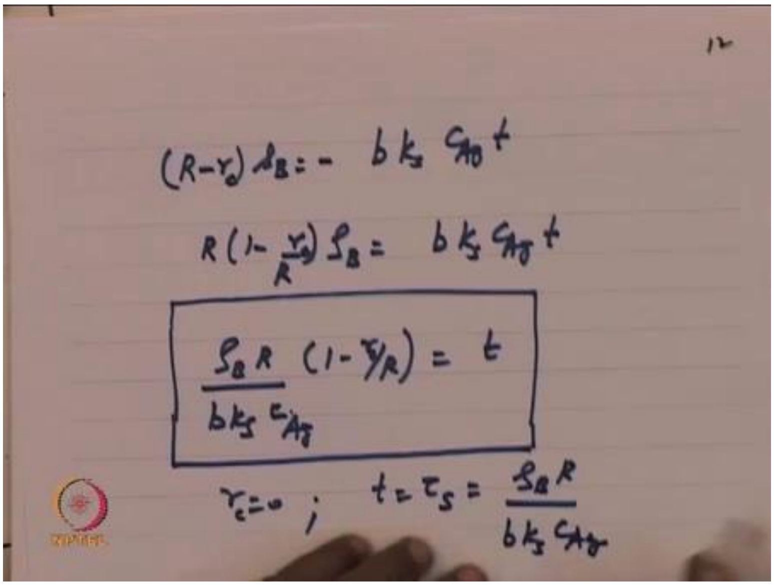

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$$(R - r_c)\rho_B = - b k_s C_{Ag} t$$

$$R\left(1 - \frac{r_c}{R}\right)\rho_B = b k_s C_{Ag} t$$

$$\boxed{\frac{\rho_B R}{b k_s C_{Ag}}\left(1 - r_c/R\right) = t}$$

$$r_c = 0 \; ; \quad t = \tau_s = \frac{\rho_B R}{b k_s C_{Ag}}$$

R minus of r times rho B equal to minus of b k s c A g t, t should come here because integrating. So, taking R common 1 minus of r by R rho B equal to b k s c A g t. So, you have rho B R divided by b k s c A g into 1 minus of r by R equal to time. So, what we get here is for the case of reaction control, for the case of reaction control the time required for consumption to any extent of reaction is given by this, Therefore, when r equal to 0, we have to put r c here, this is r c here to indicate there is shrinking core. So, r c is equal to 0 becomes, t becomes tau reaction control which is rho B R divided by b k s c A g.

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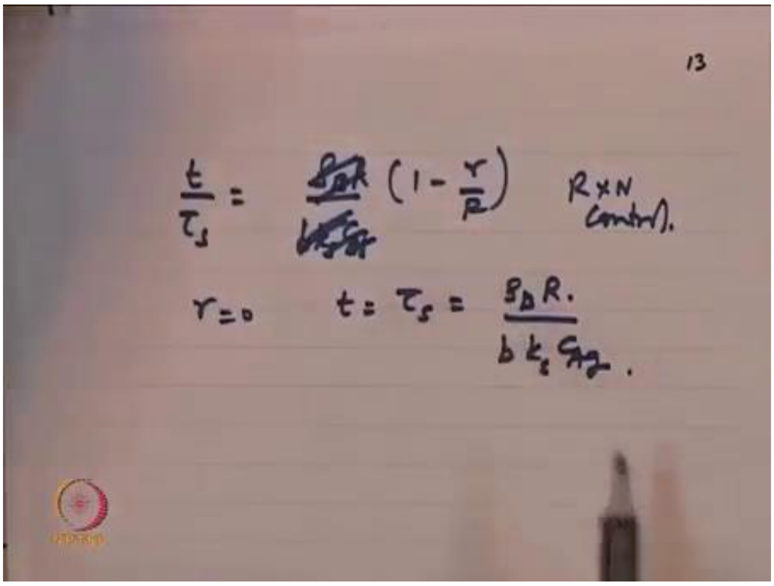

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$$\frac{t}{\tau_s} = \frac{\cancel{\rho_B R}}{\cancel{b k_s C_{Ag}}}\left(1 - \frac{r}{R}\right) \quad \text{R×N Control.}$$

$$r = 0 \qquad t = \tau_s = \frac{\rho_B R.}{b k_s C_{Ag}}.$$

So that what we get here ism for reaction control the expression for the effect of time t by tau f its tau s equal to rho b times B k s c A g times 1 minus of r by R. So, this is reaction control, what are we saying? The reaction control, the time required for any extent of reaction, to time required for complete consumption is given by the right hand side. At r equal to 0 we know it is full consumed therefore, the time therefore, t becomes equal to tau s that is equal to rho B, rho B R, rho B R divided by b k s c A g. So, what we have saying once again just repeat what we have said. We have said that this is the relationship that explains reaction control.

So, when r equal to 0 which means the particle is completely consumed, which means r equal to 0 means then this rho B R, k s b s k s become the time required for complete consumption. Therefore, this whole term can be written as tau s t divided by tau s is equal to 1 minus r by R, this what I have written.

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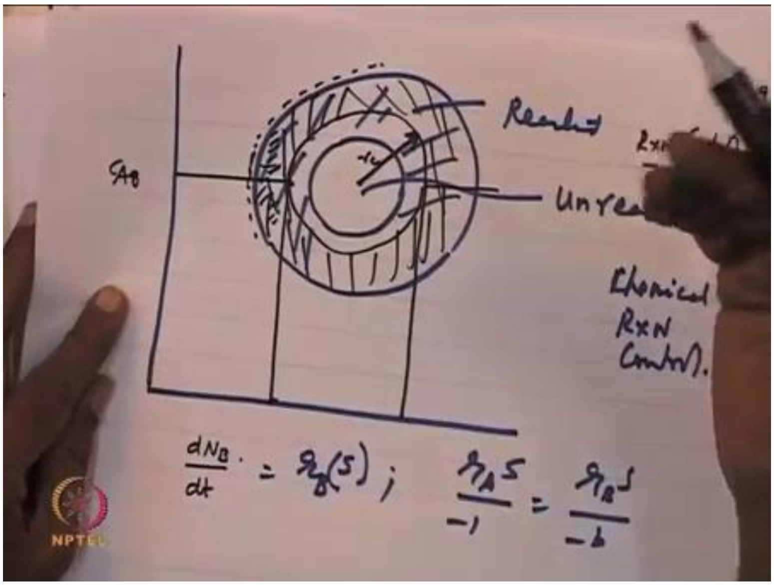

Notice here, notice here that the as a reaction proceeds, as a reaction proceeds, this point the surface which is in contact with the gas, concentration of that point is taken as 0. If he given ((Refer Time: 29:05)) then, that assumption is not correct and then, we have already developed procedure to take care of all that. So, what we have done we have taken two cases so far.

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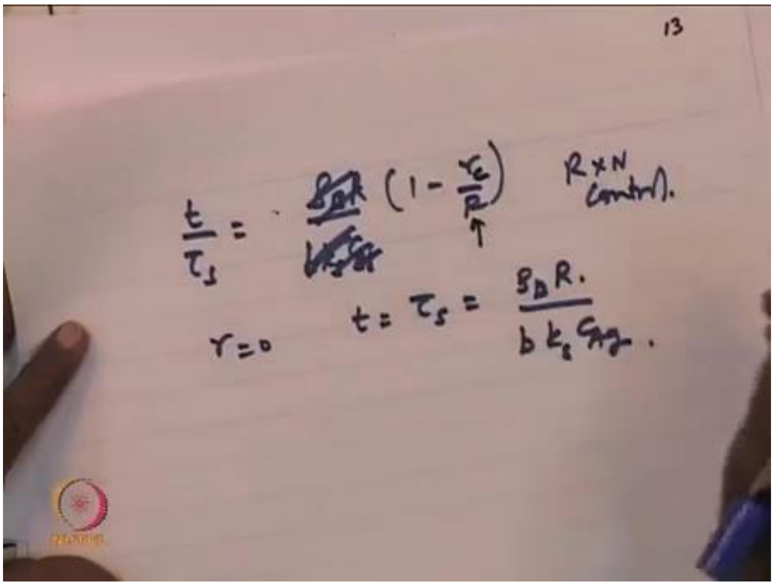

First case is when there was external film diffusion control, second case is the case of reaction control, for which we have both derived what is t by tau f or t by tau f, which is in terms of r c, which is unreacted core and then, r is the size of the particle.

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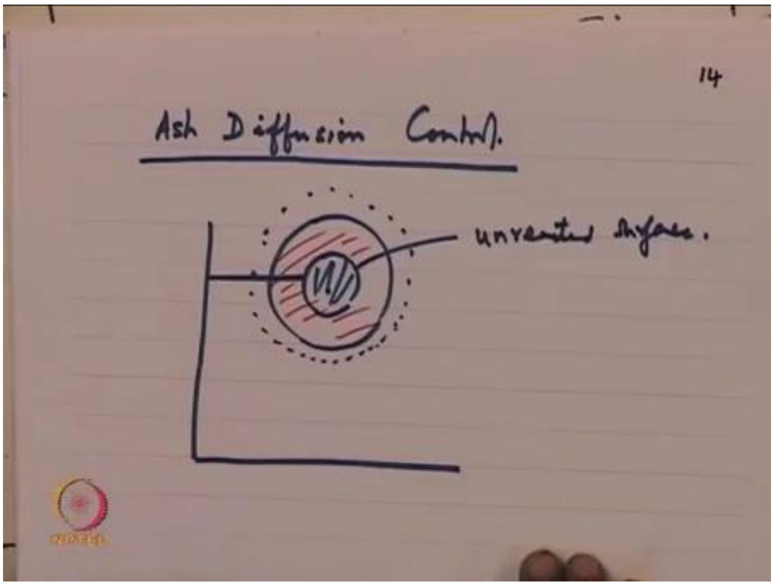

Now let us look at the third situation which is what is called as, third situation of interest to us is what is called as ash diffusion control. What we are trying to say here is the following we have a particle, we have what we call as the unreacted core and outside the unreacted core we think and there is a lamina, there is a film which is the external film.

Now what we expect is the following, as a reaction proceeds, as a reaction proceeds this is the unreacted layer and this is the, this is the reacted layer. And now the, this distance between the unreacted and reacted, this thickness keeps on growing as a reaction proceeds.

That means, as a reaction proceeds the thickness of the reacted layer keeps on increasing. So and we have to say that the reaction takes place, reaction takes place at this unreacted surface, unreacted surface which means what? As a reaction proceeds that the diffusion path around which this gas much diffuse before reaching the solid surface keeps on increasing, this an instant we should keeps understand. Now for this case let us see how to solve so that we can understand what is the rate of chemical reaction. How do we do this? We do this by recognizing the following.

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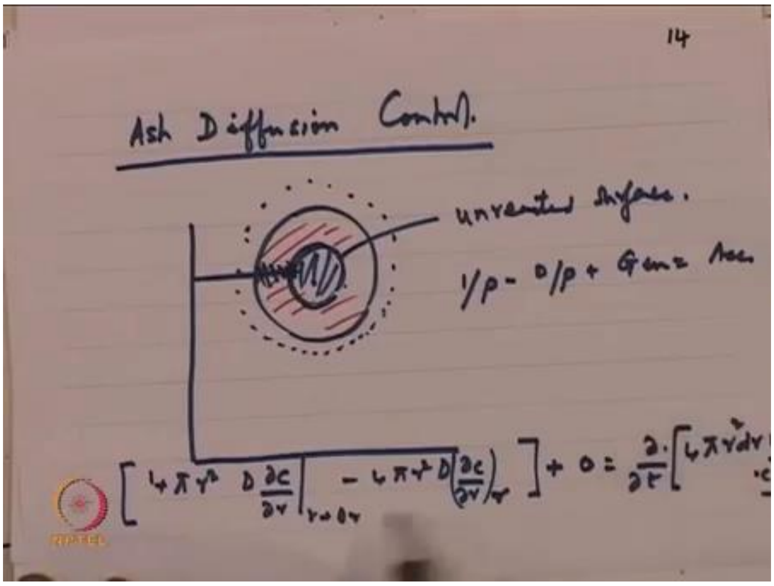

We know d N B by d t equal to r B s, we know this. You also know minus of r A times s equal to minus of r B times s equal to D times del c del r into 4 pi r square. What do we mean by this relationship? What we mean by this relationship is that, in the case of ash diffusion control the rate at which the chemical reaction takes place would be the rate at which the material arise of this solid surface. That is the meaning of reaction control, control means what? The entire process is governed by this rate of supply. So, in other words here is an instance where the rate of supply through the reacted layer is what we determine the rate of chemical reaction.

So, we must account for it appropriately so that, we can appropriately put these numbers in our equations. Let us see how we do this, what we set so for is that the unreacted layer, the unreacted layer is here, the reacted layer is here. So, this driving force which is column of these reacted materials is what determines the rate of chemical reaction. So, we must take that into account that resistance in to account to be able to handle this problem. Now, what is a general situation, the general situation is that this is a case in which we have continuous diffusion of particle, diffusion gas at the same time shrinking of these particles.

We have an instance where the diffusion of gas through the product layer, simultaneously at the solid surface the reaction is taking place. So, we have to take all these things into account, which will try to do by righting the material balance for what is going on. Let me put the material balance like this, input minus of output plus generation equal to accumulation. So, we are writing the material balance for this gas in this so, what are the inputs? Our inputs are 4 pi r square D del c del r at r plus delta r minus of 4 pi r square D del c del r at r.

So, this is the input correct, in this between r plus D r there is no chemical reaction therefore, there is no reaction is 0, that must be equal to del by del t of 4 pi r squared d r epsilon times del c del t times c, sorry. Here also multiplied by c, what have we saying here? What we saying here is that the unreacted layer, this is the reacted layer, the red one is a unreacted layer. The rate of supply of gasses to the surface depends up on resistance here, that is what we have taken into account and that is, that difference is the accumulation.

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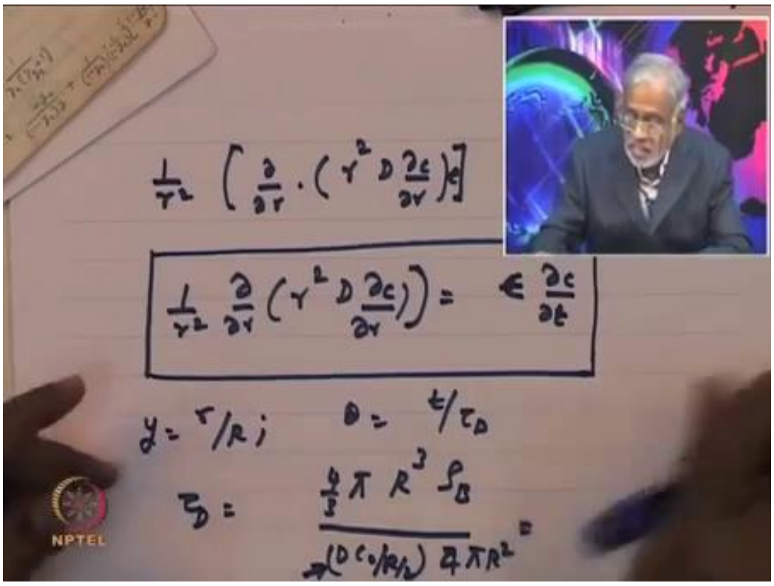

$$\frac{1}{r^2}\left[\frac{\partial}{\partial r}\cdot\left(r^2 D\frac{\partial c}{\partial r}\right)\right]$$

$$\boxed{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D\frac{\partial c}{\partial r}\right) = \epsilon\frac{\partial c}{\partial t}}$$

$$y = r/R; \quad \theta = t/\tau_D$$

$$\tau_D = \frac{\frac{4}{3}\pi R^3 \rho_B}{(D C_0/R/2)\, 4\pi R^2} =$$

So, simplifying what we get is 1 by r squared del by del r, r squared D del c del r multiplied of course. So, this gives you the accumulation of gas in this system. So, simplifying we get 1 by r squared del by del r, r squared D del c del r equal to epsilon del c del r del c del t this epsilon. Make sure all the terms are correct, 4 pi r square cancels off, 4 pi r square cancels off. So, this becomes D del c del r 1 by r squared D del c del r with a minus sign. So, no minus sign r plus d r no minus sign, epsilon del c del t. So, this is the point of writing this is the following. What we are saying this is the following, what we are saying is that in the case of ash diffusion control, the resistance to all the resistance lies in the, in this layer of, in this red layer, all the resistance lies here.

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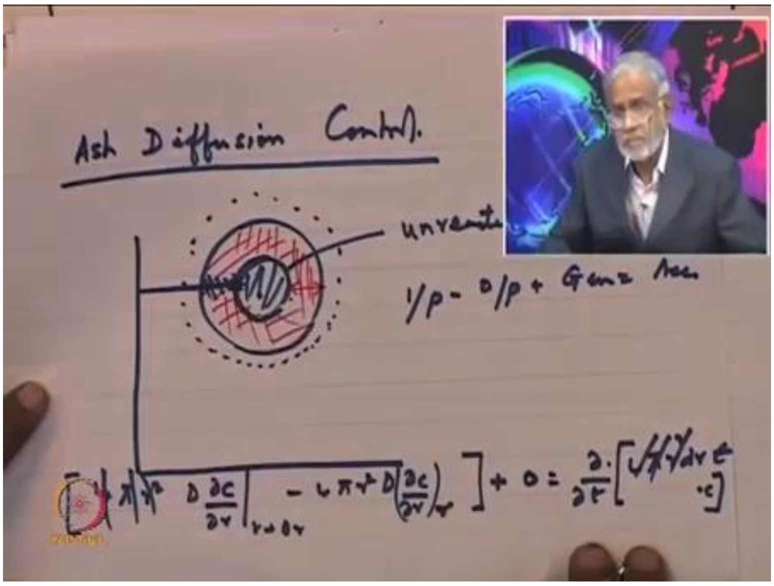

Now, as a reaction proceeds this thickness, this thickness will keep on changing. We have said un correctly that the rate of chemical reaction, rate of chemical reaction is minus of r A s or which is r B s its of minus b, already taken. So, r A s and r B s are related therefore, minus of r A s into b equal to minus of r B s. This is something we know come stoichiometry. So, what we have saying know is that the rate at which chemical reaction occurs at this solid surface can be given, can be obtain from this equation which tells us the variation of c with respect to r. So, what we have done is that we have looked at an unsteady state problem and made certain simplifications.

Let us see what the simplifications are, the simplification we would like to do is to do non dimensionalisation r by R theta equal to t by tau D and tau d we might ask how I came to this kind of formulation. Let me explain how it comes becomes very easy, D c 0 by R by 2, this is R by 2 into 4 pi r square. Now how do we understand this term tau D equal to 4 by 3 pi r cubed rho, what is 4 by 3 pi r cubed rho? This is a total mass of material there is been put into the system, what is the denominator, denominator D c 0 this term t c 0 is the maximum diffusive flux.

Because, c 0 is a concentration at the inlet therefore, t c 0 is the maximum diffusion flux divided by, what is the path length? The length is the path as you can see here, our path length is at best R by 2, this is the R by 2. So, this is our path length of R by 2 is chosen so that, we get this tau D is the total amount of material is divided by a diffusion which is D c 0 R by 2.

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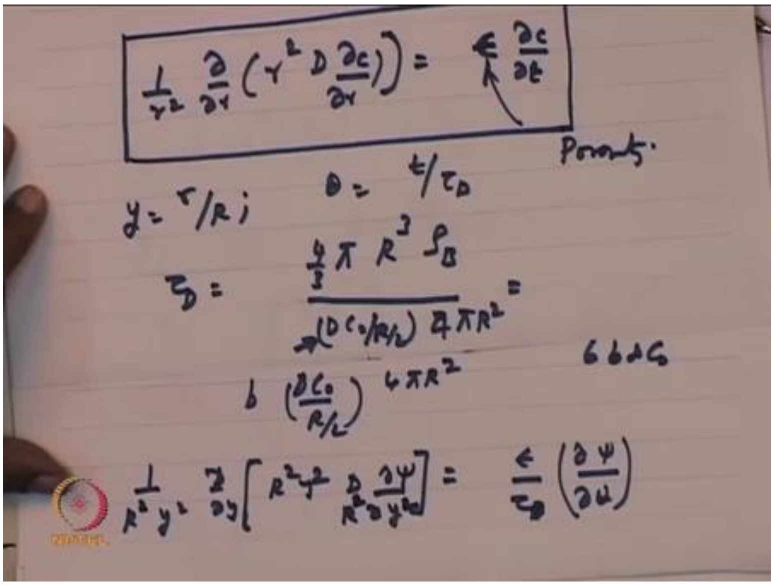

$$\boxed{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D\frac{\partial c}{\partial r}\right) = \epsilon\frac{\partial c}{\partial t}}$$

Porosity.

$y = r/R;$ $\theta = t/\tau_D$

$$\tau_D = \frac{\frac{4}{3}\pi R^3 \rho_B}{\left(D c_0/(R/2)\right) 4\pi R^2} = \qquad 6 b D c_0$$

$$b\left(\frac{D c_0}{R/2}\right) 4\pi R^2$$

$$\frac{1}{R^2 y^2}\frac{\partial}{\partial y}\left[R^2 y^2 \frac{D}{R^2}\frac{\partial \psi}{\partial y}\right] = \frac{\epsilon}{\tau_D}\left(\frac{\partial \psi}{\partial \theta}\right)$$

So, we are able to detail a priory what is the diffusion time. Now let us look at a simplification, what is the simplification that we want to do is, we want to non-divine to solve this. So, our equation is 1 by r squared del by del r, r squared D del c del r equal to epsilon del c del t. To solve this, we have what is called as the non-dimensional representation, it makes it a little easier to understand what is going on. And tau D equal to 4 by 3 pi r rho row B divided by b time 6 times D 0 by R by 2, 4 pi r square. Please let us understand what is meant by these terms, y equal to r by R this, is it is a well-known thing.

And theta is tau at this is reaction time verses the complete consumption time for diffusion control. So, with this we find that our tau D becomes this and when we simplify what is it become? Rho B R square 6 b d c 0, let us see whether all the number was correct, 4 by 3 pi r cubed, pi r cubed. Now let us look at this solution now, I want to non-dimensional lies this differential equation in terms of these variables. So, we get 1 by R square y square del by del y, del by del y which is R squared y squared D del by del y is del by del y times r, correct.

That is equal to the right hand side which is epsilon by tau D tau D del psi by del t, please understand this, what awe saying now? What we saying is that we have this differential equation 1 by r square del by del r r square D del c bye del r. Then, right hand side is epsilon is porosity, this porosity and this is time and so on. So, we have non-dimensionalised with respect to y equal to r by R and theta equal to t by tau D. So, this whole equation must now be written in terms of we our del y square. Therefore, will be r square will come del by del y, have we got everything correctly?

See, r square del c del r del c del r r is r square will not come so, let me see I have got all the terms right, 1 by r squares is correct, del y is correct del by del r. So, one more r will come so, one more r will come here, because of this r correct. So, r square y square so, d del c del r so, it is r del by del y. On the other side epsilon tau d del c by del theta, this is tau d.

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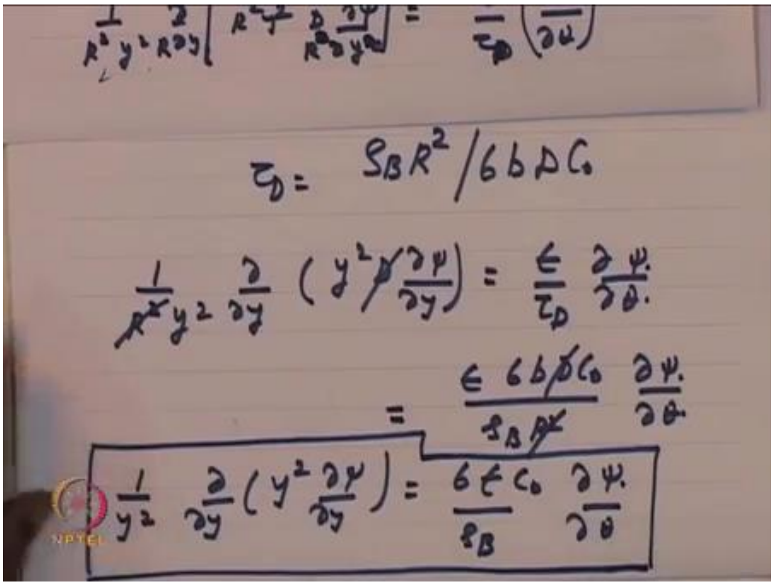

$$\tau_D = \rho_B R^2 / 6 b D C_0$$

$$\frac{1}{\cancel{R^2} y^2}\frac{\partial}{\partial y}\left(y^2 \cancel{D}\frac{\partial \psi}{\partial y}\right) = \frac{\epsilon}{\tau_D}\frac{\partial \psi}{\partial \theta}$$

$$= \frac{\epsilon\, 6 b \cancel{D} C_0}{\rho_B \cancel{R^2}}\frac{\partial \psi}{\partial \theta}$$

$$\boxed{\frac{1}{y^2}\frac{\partial}{\partial y}\left(y^2\frac{\partial \psi}{\partial y}\right) = \frac{6 \epsilon C_0}{\rho_B}\frac{\partial \psi}{\partial \theta}}$$

Let me simplify this further, what we get going from this to the next one and we can see here r square, there is a r cube. So, there is r square here so, essentially denominate there is one r here, there is one r here. Therefore, it simplify it as 1 by R square y square del by del y of y square D del psi del y, equal to epsilon by tau D del psi del theta. Now our tau D please recognize I will put it down here, tau D we have define tau D in such a way that it looks like this. Rho B R square by 6 b D C 0.

Now, you can replace tau D here so, that and this writing the right hand side only epsilon and then tau D is what? 6 B, 6 B d c 0 by rho B R square. The right hand side is del psi del theta. Now a lot of simplifications you can do from so that, now with this equation looks like this r square cancels off d cancels off and so on. So, you are left with 1 by y square del by del y y square del psi del y equal to 6 epsilon c naught by rho B del psi del theta.

This is the equations that governs what happens inside the particle. See why are we doing all this? We are doing all this just to understand an important feature of our problem. What is the important feature of our problem?

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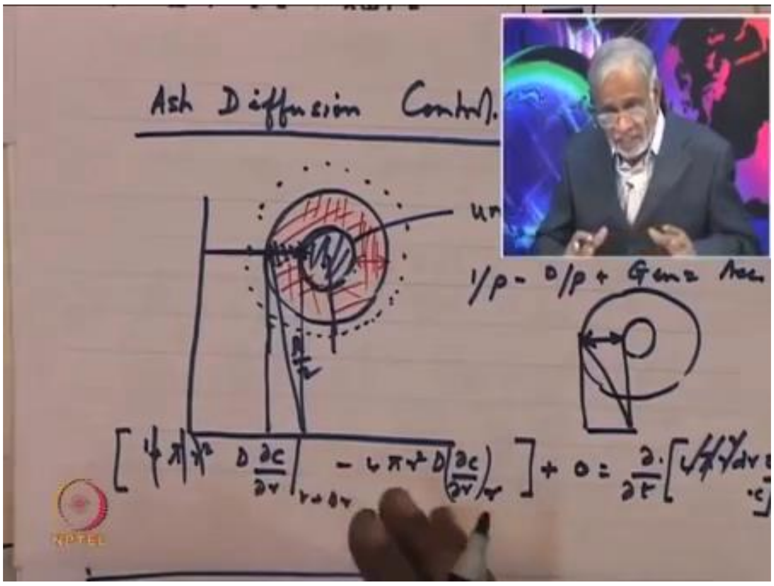

The important feature of our problem under ash diffusion control is that, as the reaction proceeds the thickness of the ash layer or product layer keeps on increasing. And our reaction the drop in concentration, the drop in concentration come from, it is c A g here and it drops to 0 here. So, it from here to he now when this when this distance is more that means, the second case so, this case the second case will drop this distance has increased. That means drop occurs over a larger distance.

On other words, our mathematical formulation must take into account this increase in the diffusion path as the reaction proceeds. What have we done for this?

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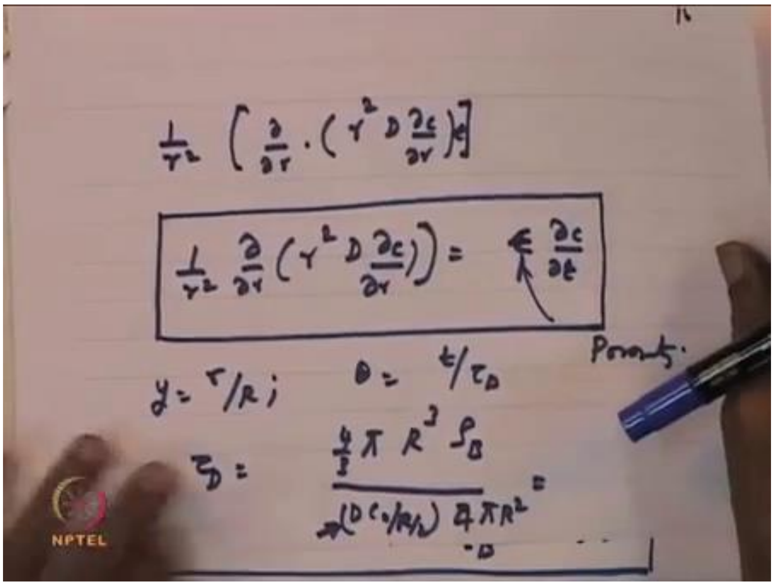

$$\frac{1}{r^2}\left[\frac{\partial}{\partial r}\cdot\left(r^2 D\frac{\partial c}{\partial r}\right)\right]$$

$$\boxed{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D\frac{\partial c}{\partial r}\right) = \epsilon\frac{\partial c}{\partial t}}$$

Porosity.

$y = r/R;\quad \theta = t/\tau_D$

$$\tau_D = \frac{\frac{4}{3}\pi R^3 \rho_B}{(D C_0/R/2)\, 4\pi R^2} =$$

What have we done for this is to recognize that our equation that describes the motion or the variations are given by this equations. Where, we can non-dimensionalise under certain conditions where we assume tau D to be this, which is the total amount of material divided by the average diffusion through this. So that, we define the average time of a what is called time of diffusion time. So, with all these simplifications we have reduce these equations to look like this.

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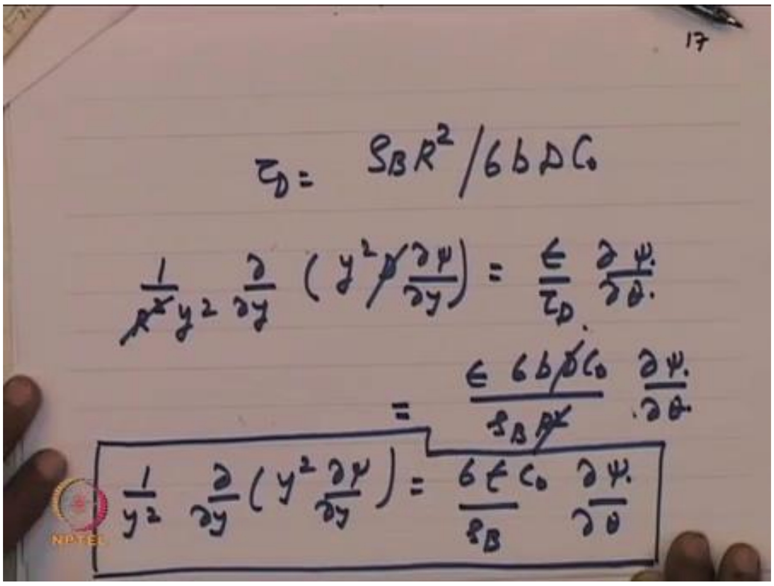

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$$\tau_D = \rho_B R^2/6bDC_0$$

$$\frac{1}{R^2 y^2}\frac{\partial}{\partial y}\left(y^2 \cancel{D}\frac{\partial\psi}{\partial y}\right) = \frac{\epsilon}{\tau_D}\frac{\partial\psi}{\partial\theta}$$

$$= \frac{\epsilon\, 6b\cancel{D}C_0}{\rho_B \cancel{R^2}}\frac{\partial\psi}{\partial\theta}$$

$$\boxed{\frac{1}{y^2}\frac{\partial}{\partial y}\left(y^2\frac{\partial\psi}{\partial y}\right) = \frac{6\epsilon C_0}{\rho_B}\frac{\partial\psi}{\partial\theta}}$$

1 by y square del by del y equal to the, equal to right hand side 6 epsilon c naught by rho B del psi del theta. Please notice that, the order of magnitude of y is maximum value y can take this 1. So, the order of magnitude of psi is 1, order of magnitude of theta is also 1. Because it is non-dimensionalised with respect to tau D. So, on the other words here is a non-dimensionalised representation of the diffusion equation through the product layer where, the multiplicative factor is 6 epsilon c naught by rho b. What is this 6 epsilon c naught by rho b?

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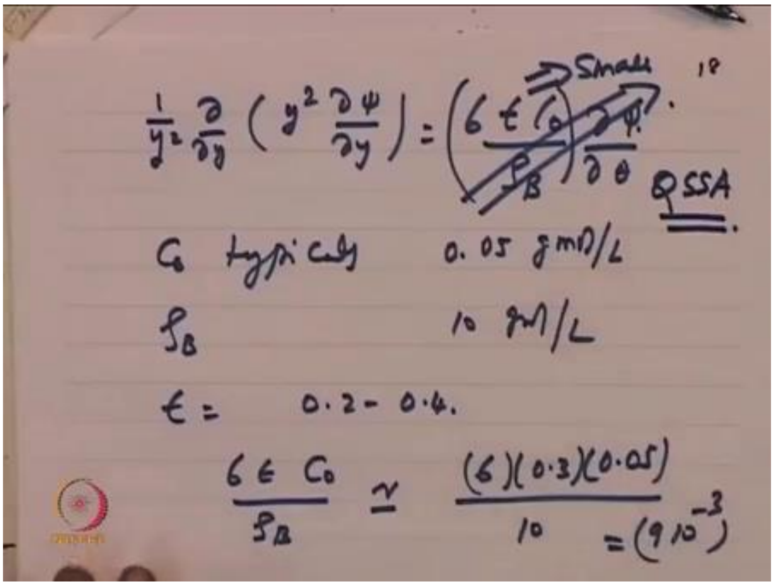

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$$\frac{1}{y^2}\frac{\partial}{\partial y}\left(y^2\frac{\partial \psi}{\partial y}\right) = \cancel{\left(\frac{6\epsilon C_0}{\rho_B}\right)\frac{\partial \psi}{\partial \theta}} \Rightarrow \text{Small}$$

QSSA.

C_0 typically 0.05 gmol/L

ρ_B 10 gml/L

$\epsilon =$ 0.2 - 0.4.

$$\frac{6\epsilon C_0}{\rho_B} \simeq \frac{(6)(0.3)(0.05)}{10} = (9\,10^{-3})$$

You know from ours experience, we know the following. What we know? We know that that c naught so, let me write this equation once again. 1 by y square del by del y y square del psi del y equal to 6 epsilon c naught by rho b del psi del theta. Now c naught typically so, about 0.05 gram-mole per liter, we know this. Rho b for solids is typically 10 gram-moles per liter. So, what we saying is and epsilon is about 0.2 to 0.4 shall we say. So, this whole term 6 epsilon c naught by rho b, we can calculate 6 multiplied by 0.3 let say is 0.18 c is 0.05, 0.18 multiply 0.05 divided by 10.

So, you can see here this number is a small number. On other word the this term 6 epsilon c naught by rho b this is approximately, I will put the numbers here you please calculate 0.3 0.05 divided by 10 equal to. So, we can see 0.3 0.3 0.09 something like 9 10 minus 3. So, this is the value it takes, is it correct? 6 into 0.30.3 0.09 0.009. So, about 10 minus 3 so, this is small number, what you want to say here is that this quantity is small, this is small. So, what is it mean, it means that under the conditions of the formulation of the problem, it is possible for us to delete the right hand side.

Saying that the right hand side is not very important, it goes to 0 or this is what is called also call quasi steady state approximation that means, accumulation of material inside the particle as the reaction proceeds is small. Therefore, we can as well assume that the left hand side is approximately 0.

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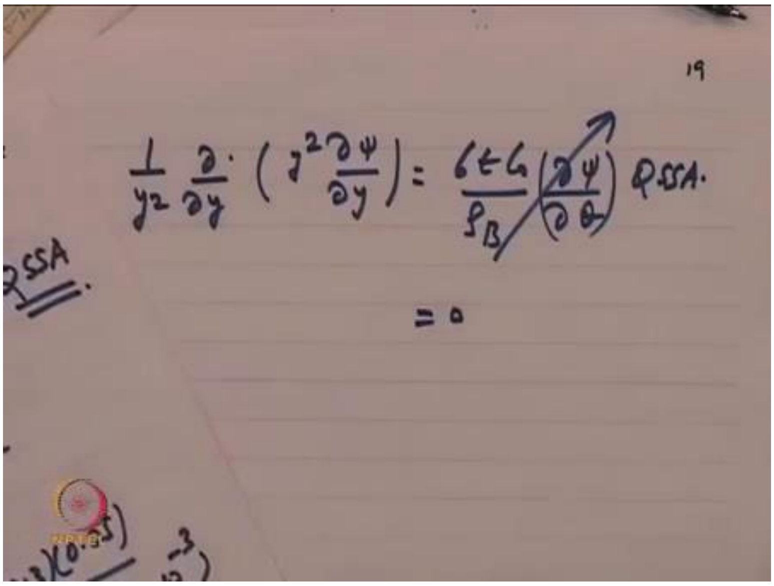

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$$\frac{1}{y^2}\frac{\partial}{\partial y}\left(y^2\frac{\partial\psi}{\partial y}\right) = \cancel{\frac{6\epsilon C_0}{\rho_B}\left(\frac{\partial\psi}{\partial\theta}\right)} \quad \text{Q.SSA.}$$

$$= 0$$

QSSA.

So, our problem therefore what we are trying to see here that, this 1 by y squared del by del y, y squared del psi by del y equal to the right hand side 6 epsilon c naught by rho b del psi by del theta. This is not very important, this is what is quasi steady state approximation. Therefore, we might as well solve this problem by assuming that 1 by y square del by del y y square del psi del equal to 0. This would be a satisfactory way of understanding diffusion of gas through a solid particle under the condition quasi steady state approximation.

On the other words to understand the rate at which the reaction would take place, over the solid during the instance of ash diffusion control we might as well solve a simple of problem 1 by which is essentially quasi steady state approximation problem, which give us answers which are quite satisfactory. We will take this up, we will be meet next.

Thank you.