Chemical Reaction Engineering II
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Lecture - 9
Introduction to Intra particle diffusion

Good morning. In the last lecture, we look that how to derive or synthesis a rate law for heterogeneous catalyst, when the reaction is taking place in the surface. The different steps occurring while the reaction taking place on the surface of the catalyst. We already look that these steps. First is of course, the external mass transfer, then the internal mass transfer or diffusion to the force and actual catalytic side is present on the surface which are nothing which is nothing but the wall of the pole and on this side reaction would take place.

So, after the diffusion that is the second step, we have adsorption of the reactant on the catalytic side, and then the adsorpt species or the adsorpt component will undergo the reaction. We looked at isomerization, dehydrogenization reaction, there are many possible reactions. And this transformation will occur on the surface that is nothing but a surface chemical reaction. Then the product which is possibly in the adsorpt state will get dissolved the force step and, then aging in the back diffusion through the force of the part of the product. And then the external mass transfer of the product.

So, these are the different steps, we already look that them. But while deriving the rate law, we look that only 3 steps that is, adsorption, surface reaction and desorption. Only 3 steps we look that and we synthesis the rate law. And then I told you how to determine, how to validate this rate law or in the sense, how to know whether the rate law get we have synthesize is correct or not. That is through the experimental data, performing experiments in laboratory. And the different conditions and seeing the effect of partial of the reactant; some time the product and see whether the rate equation that we have derived, fits well in the experimental data that we have got.

So, I give you 1 example last time of a cyclohexane dehydrogenization. And I told you how it fits well for the rate equation derived base on the assumption; that the chemical reaction controls. But sometime it quite possible that, adsorption desorption would control. So, it all we have to check that through the experiment. Now, today we are going to look at the other steps, which we had ignored before and these are external mass transfer and internal mass transfer that is diffusion. So, we going to spend some time on diffusion 1st right and then we look at external mass transfer.

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So, on a catalyst practical, we have reactant going force to the external surface, then inside and some were you have catalytic side; whether adsorption reaction and desorption occur and then the feedback diffusion and then back mass transfer to the bulk of the product. So, these are the steps. We are now going to concentrate more, next 3 4 lectures, on this particular steps that is pore diffusion; a very impotent step. I told you that, the catalyst are poresive nature and they are different of them many several pores in the catalyst. In fact that is a main reason; the catalyst would have very large surface area.

So, even if the main active catalytic components say for example, palladium or platinum or nickel or ruthenium. These metals may not have very large surface area, what we do is; we put they on supports. Supports have very large surface area, we disperse this catalyst on the support, so that we get very large surface area and nice dispersion, maximum number of atoms of the catalytic component will be available for the reaction and I need very less catalytic loudly. That is a idea.

So, we are going to look at the pores catalyst now. As a told you before the first lecture on catalyses, they get different types of catalyst. Sometimes of you may have to deal with non pore catalyst, with the reaction takes place only on the external surface, like for example, gauss a platinum gauss, a silver gauss and all that. In that case we do not need to very about this pore diffusion effect. But, there are many catalysts which are pores in nature, for them we need to consider the effect of pore diffusion. The rate equation that we are derived, we further get modified, because of the pore diffusion effect. And we are going to a look at the effect of pore diffusion in this particular lecture. Now I have told you that we have catalysts.

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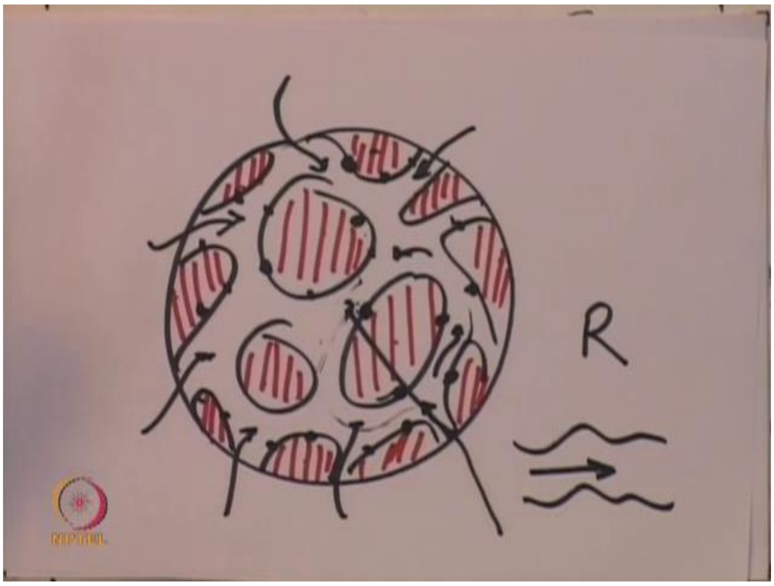

I will re draw the picture of the catalysts again. So, we have this catalyst, in which you have to different pores. Remember, I had done this before as well write. And then I have this particular space, which may be considered as solid container solid. Actually there are micro pores inside, but than for over analysis purpose, let say that I have these spaces were only solid is present and this are the empty spaces which are nothing but pores. And the actually catalytic side will present somewhere on these surfaces or the wall of the pores. And in order to access these sides a molecule has to diffuse right.

So, it will enter the pore from various locations. There be serve such location true which it will go inside and get diffuse. So, if the catalysts particle has a radius R, overall movement of the reactant molecule will be inside catalysts particle towards the center. Though it will not directly go to the center, because there is huddle here, constriction here all right, it will go this way. Why I am explaining all this in detail, because later on we are going to consent called effective diffusivity and good related to the normal diffusivity, when with a molecule is moving without any constriction hurdles and so on.

Now, imagine a situation, where I have a molecule which is sitting in the center of the; this class room. And for some reasons, it is a concentration gradient molecule has a diffuse right. Diffusion takes place when you have a concentration gradient, all other chemical potential gradient and it has to diffuse. Now this molecule, does not know where the walls are, walls are far away from the molecule. And this molecule will flow assuming or other will get transferred rather. Then you flukes because of it is movement right. Assuming that are no walls at all, because they are far away from the molecule.

Now what is this particular motion molecule, like how do we characterize, it is a fix law right. And then there is a constant called as diffusivity. This diffusivity has nothing to do with the walls, it is a free molecule present in the bulk right and it is moving right, because concentration radiant. Now this is not good experience any resistance otherwise, from the walls, but there will be some resistance and because of it is molecular way, because of media and all that. And that is why we have called we have a parameter called diffusivity. And this diffusivity will decide how fast the molecule will move.

Now compare this situation as against, the molecule which is present inside the pores. Now if molecule is moving here, it is going to experience some resistance from the walls why, because look at the pores; what is the typical size the pores? The pore size is very small and that is the reason we get a such a last surface area. So, this size is of the order of few nanometers or it can be and strong. There are different types of pores; micro pores, macro pores, meso pores, a very small. And the order of the magnitude of this diameter of pore, is comparable is the size of the molecule. What is typical size of the molecule? Say benzene, it is close to 6 anxstorng. So, 6 anxstrong molecule size and suppose you have a pore of say 15 or 20 anxstorng, then it is going to definitely face some resistance. Look at main free path or the molecule, definitely it will experience existence of the wall around it and the diffusivity will go down.

So, this wall effect, what else there is, for example, this molecule is moving from the external surface inside. If I look at actual distance travel by the molecule, it is this distance, but the molecule is going go this way right. So, it has to follow a torches path and the diffusivity, the effective diffusivity, if I considered the actual moment this, then the diffusivity will further go down, because of this path that it has to follow. For the same displacement or the movement or distance, it has to go this way right. S

o, this is another effect. We are going to put all this effect in 1 parameter later. Then, the pores these pores there is no guarantee that there should be a uniform size. There are few catalysts especially geo light and all that, where the pore size is well defined. But take example of iron exchange of resign, you cannot defied the pore size, it is in the range. There is a pore size distribution the deal see right. So, if you take single pore, the pore itself will have something like this. The wall is not straight. And then there is the possibility that, the area of cross section will vary as the molecule moves ahead. So, there is again some constriction that it is going to experience right. And because of that, further the diffusivity will go down. So, now the effective diffusivity, if I want to determine the effective diffusivity, that diffusivity is nothing but the normal diffusivity and the effect of all this factors. So, let us define term called effective diffusivity.

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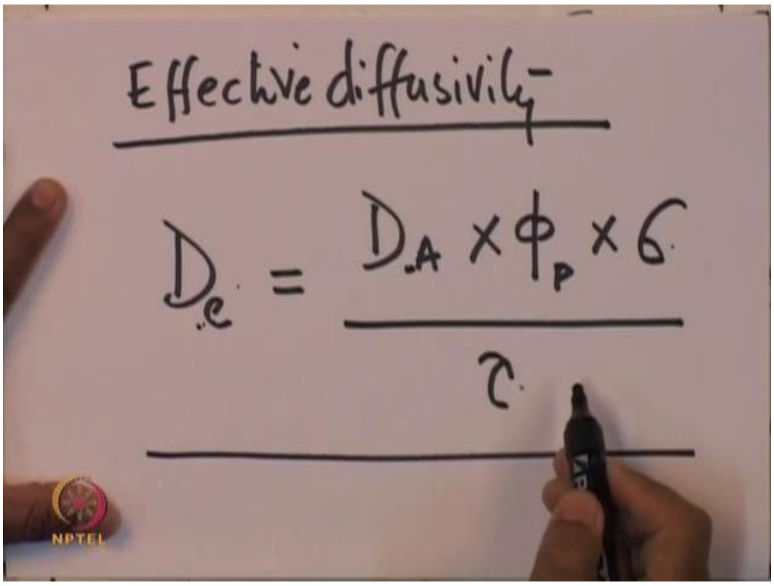

Effective diffusivity

$$D_e = \frac{D_A \times \phi_p \times \sigma}{\tau}$$

So, we call this is D e effective diffusivity. Effective diffusivity is equal to nerson diffusivity D a, which is the diffusivity inside the force. That menace, it considers the resistant of or by the fluid inside the pore and the walls of the pores. Now, how do I relate this 2? This is definitely going to be larger than this, because this is smaller right. So, they are some effect, because there is a space constraint. So, some effect will come because of phi p which is nothing but porosity. Because, some space is occupied by solid, that is not available for the movement right of the molecule. So, it has to be multiplied by the porosity. Porosity is always less than 1.

Then, I was telling about the constriction, this is called as the constriction factor, because the variable area. And there is another factor called as torchesity all right. Sometime we club this 2 and I called like the torchesity factor. In some books, we will see sigma not present there and you have a tau a f for whatever torchesity factor. But what needs to be understood from this is that, this in normal nuts and diffusivity that we defined for a molecule right. You have phi here, taking effect of considering the effect of porosity, presents of solid constriction and then the torchesity. This considers the effect of wall anyway. But these 3 factors are the factors which are dependent on the solid that we have. It is the morphology; it is pore of stature and so on.

So, these are the factors which will change from particle to particles, solid to solid, catalysts to catalysts right. So, this is the effective diffusivity. Now this diffusivity, once I have this, I have this diffusivity in terms of other factor. I can right in normal fix law types of equations for a solid pore solid. So, what this allows is; doing is to right mass balance flux equation based on fix law. Only difference is instead of a normal diffusivity, we have a effective diffusivity here. Now let us spend some time understanding torchesity.

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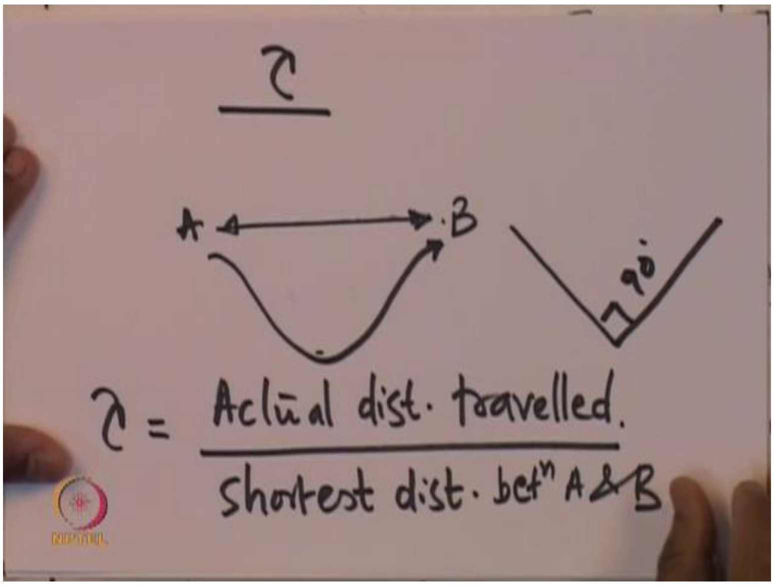

$$\tau = \frac{\text{Actual dist. travelled}}{\text{Shortest dist. bet}^{n}\text{ A \& B}}$$

Now this tau that we have defined is as I said like the molecule has to follow a path this way, because of the pole structure, but actual distance when it travels is only this much. So, I made extra surface, I am going inside, but we need to follow this path. So, the extra path that it has to follow will result in reduction in the diffusivity. Now the torchesity is defined as; actual distance travelled divided by shortest possible distance between this 2 points. Suppose this point A, this point B is shortest possible distance between A and B right.

So, it is very easy to define or even easy to calculate the value of tau. Suppose I know the angle here. So, let say I have I adjust I approximated like this. And this is say 90 degrees is a angle. Can I calculate value of torchesity? You can do this exercise.

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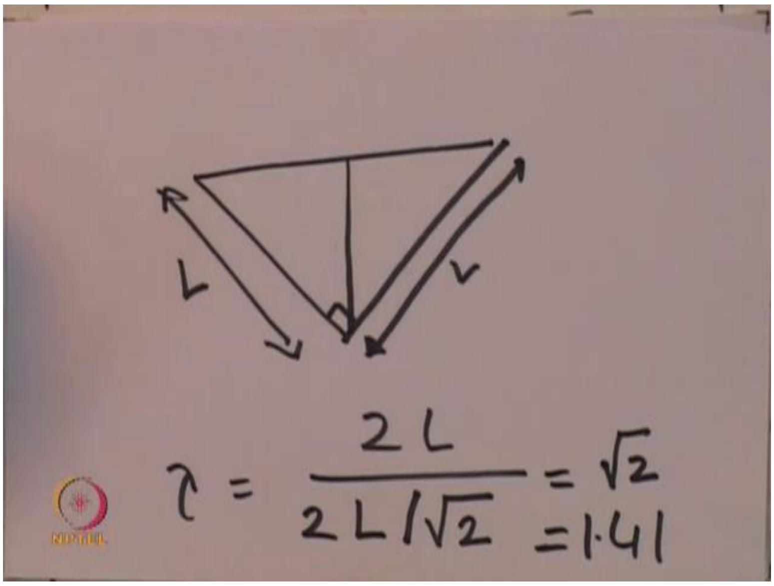

Torchesity is the actual distance travelled. So, let me say that, this is L, this is L. So, the actual distance travelled is 2L. If this is 90, then again calculate distance, this going to be 2L divided by root 2. So, the value of torchesity comes out to be root 2 which is 7.41. The torchesity is greater than 1; it is always greater than 1. We cannot expect to have straight pores, very difficult. So, an extreme situation would be torchesity is 1, but quit unlikely. Sometime the torchesity can be of the order of 5 6 7 10, it can be that high, it all depend on material. And of course, people have control or making the material also like; this is separate at all together different area, where we design catalyst as per our requirement.

But then for our analysis, let us take this torchesity as a material property. And that we come when the or that can be evaluated, when the material is designed or it is available. And, then we go head and a value of effective diffusivity, based on the known value of nuts and diffusivity. Now once we know the value of diffusivity, as I said before we can write the fixed law for the solids.

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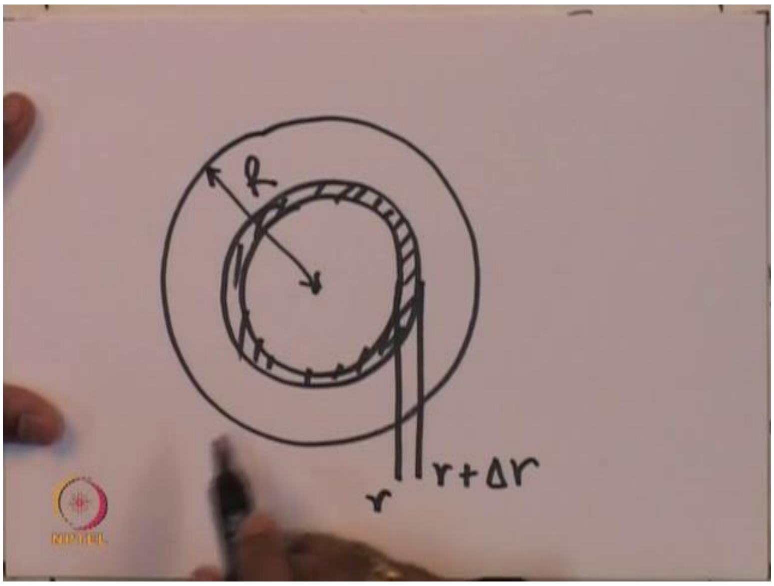

So, let us assume that, I have a spherical particle and then the molecule is going inside. Now, this is the center and let us take a differential element and write fix laws around this. So, this is r plus delta r and this is r. And the radius is R. Now this is the diffusion taking place. As I told this particle go to have pores inside, but now I am got assume, that the diffusion is taking place straight along the radial direction. Actual movement like this, but then now that I have considered that, effect of torches movement, in my effective diffusivity I am free to write equation, something similar to what I do. Normally for diffusion or flukes writing mass balance, when there is a concentrate guide.

Now, look at this particle again; this is catalysis happening. Inside the reactions taking place, so assignment molecule goes inside, it is go to meet catalytic species and reaction go to take this. So, it is something happening parallel. So, reaction and diffusion and they are taking place simultaneously. So, assignment there is movement, the reaction of the taking. Now, overall rate the reaction, we will depend not only on the actually rate of reaction, actually in the since 1 that we derived yesterday, considering effects of absorption, desorption and chemical reaction whichever is a controlling, whatever that particular rate and now the rate of diffusion will also matter.

You can imagine a situation, where the reaction instant; very fast. Even if absorption control or desorption controls are even the reaction can chemical surface reaction, all this steps are happening very fast. But, then diffusion becomes very slow, that party slow molecules are not able to defuse inside, then the overall rate will go down. So, diffusion is playing an important role here. If the diffusion is very fast, the pores are wide enough, diffusivity is very large, then it is a chemical reaction or whatever; absorption, desorption at the site that we probably control over all rate. So, try understanding part of diffusion now internal diffusion. We are not talk about external diffusion external diffusion mass transfer.

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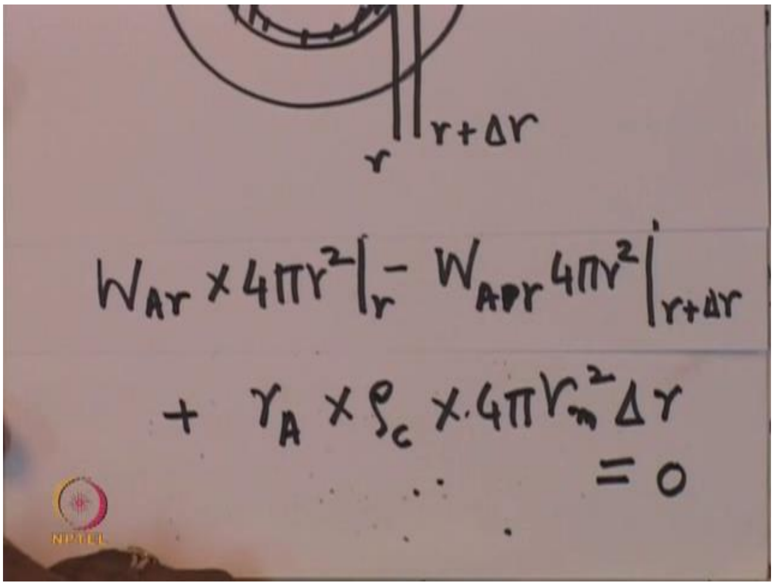

$$W_{Ar} \times 4\pi r^2 \Big|_r - W_{APr} 4\pi r^2 \Big|_{r+\Delta r} + r_A \times \rho_c \times 4\pi r_m^2 \Delta r = 0$$

So, we are going to write the law the mass balance. For this the flux balance, there is no convection here, is only diffusion that is taking place. So, the flukes at r is W A r. This is the way I am defining the flukes, W the flukes of component A that this reactant in radial direction, into 4 pi r square, what is it, in the area right, at r at r minus W A r 4 pi r square at r plus delta r here, the flukes here minus the flukes here, can I write this equal to 0? No right. This is another term that we need to consider here. What is that term? That term is reaction. If there is no reaction, then this would be called to 0, but there is reaction taking place.

So, look at this as a CSTR, material coming in, going out and plus reacted is equal to 0.

So, I need to add the reaction term. So, plus reaction rate r A into let me explain all these later, first let me write into row c which is nothing but the density of the particle mass per unit volume into 4 pi r m square into delta r. So, this is reaction term, I will explain in this detail, is equal to 0.

So, material at r going out minus coming in plus generation term and now r A will have it is own sign, depending on whether we have reactant product, were is a reactant there is a negative sign. What is this? This is volume; this is volume 4 pi r m square into delta r. Then, row c is a density. So, this is volume, this is density, then density into is volume is nothing but mass. So, rate is express per unit mass of the catalyst. I told in the last lecture, most of times in solid catalyst a reaction, the rate is expressed per unit mass of the catalyst.

So, r A is per unit of the catalyst, you have to multiply by the way. So, this is to be, this has to be in the watt of the catalyst; so density into volume. So, this is the mass balance. Now let us go ahead and try and elaborate this term called W A r which is nothing but flukes. As I said we can use fix law for this with a spherical coordinate, to write the flux equation for W.

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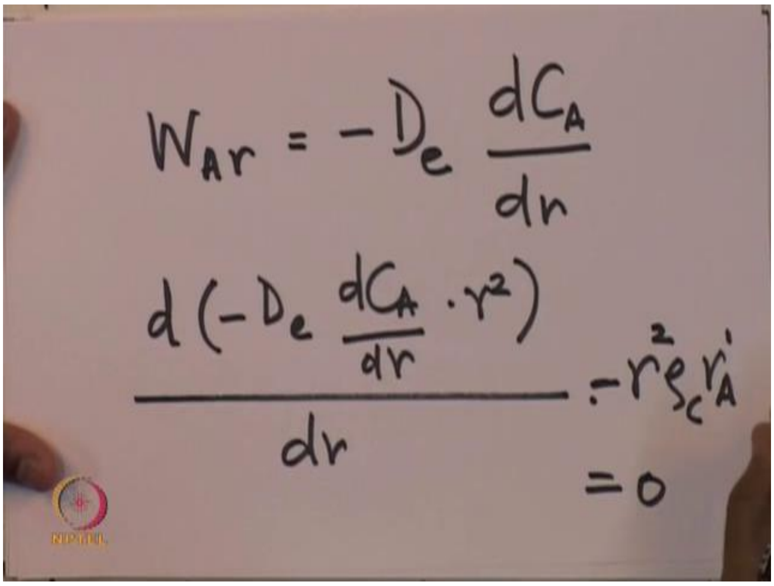

$$W_{Ar} = -D_e \frac{dC_A}{dr}$$

$$\frac{d\left(-D_e \frac{dC_A}{dr} \cdot r^2\right)}{dr} - r^2 \rho_c r'_A = 0$$

So, W A r is nothing but minus D e, that is, effective diffusivity into d C A by d r. So, this is flukes, now it substitute for this flukes in the main equation, then what do we get? We get and of course, like we have r and we have r plus d r, then just play with the equation, assume delta are approaching 0, I can convert that difference equation to the differential equation. And then what I get is this d minus D e d C A by d r into r square divided, but this is d by d r of course, is minus r square row c r A dash is equal to 0.

So, I just substituted for W and converted different equation to the differential equation and I get this particular equation. Now, if I want to write a expression for r A dash, what is r A dash? r A dash is rate of reaction, intrinsic of reaction when the molecule is present near the catalytic sight. So, if r A, we can obtain it by rate law, then r A can be k into C raise to n.

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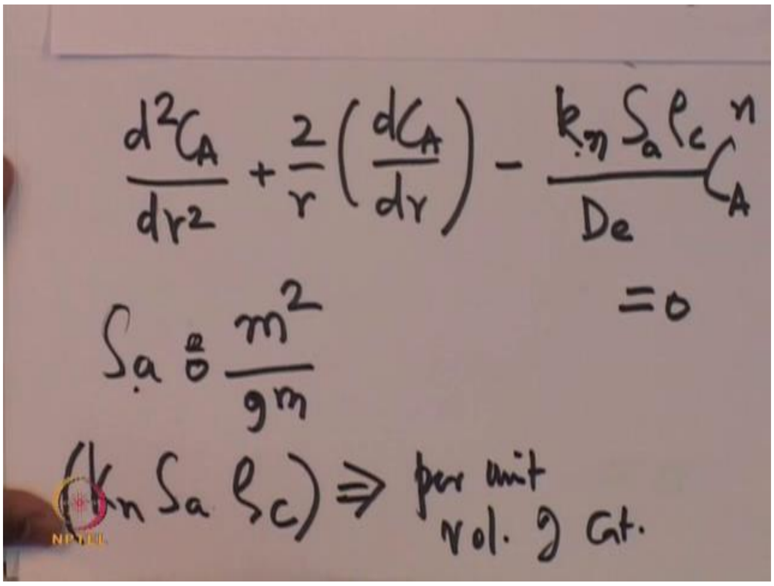

$$\frac{d^2C_A}{dr^2} + \frac{2}{r}\left(\frac{dC_A}{dr}\right) - \frac{k_n S_a \rho_c}{D_e} C_A^n = 0$$

$S_a : \frac{m^2}{gm}$

$(k_n S_a \rho_c) \Rightarrow$ per unit vol. of Cat.

So, if I expand it further, what I get is d 2 C A by d r square, this expand is further plus 2 by r d C A by d r. Let me explain it later, but let me write it first; k n into S a into row c divided by D e. Look at this D e, D e is coming here, I am just dividing both the terms by D e right, that is, effective diffusivity into C A raise to n is equal to 0. Now, you would able to guess what I have done here, I have divided both the sides by r square right.

So, what is happening is; in you have d 2 C A by d r square second order equation, d C A by d r 2 by r. Now, I have little expression for r a dash, that is, the rate of reaction at the catalytic side in terms of these concerns. So, let us try to understand this constraints; k n is going to be the rate constant which is the units, then S a is a surface area is a surface area, row c I have already told you it is the density mass per unit volume, C A is a concentration raise to n, this n is nothing but order of the reaction with respect to A.

The intrinsic kinetics here has been assumed to be length order reaction. Let me the kinetics is the power law model, rather than the commonly used models like and so on for heterogeneous catalysis. I have a reaction, this say it have only ah an isomerization reaction a going to b, only single react represent. So, k into C A to strength and this is nothing but diffusivity.

Now can you this unit of k m? I have multiplied it by surface area now. So, now, this surface what is S a? S a is a surface area. Now what is a unit of S a? S a is a say meter square per gram of the of the catalyst of the kg of catalyst whatever. So, this is unit of S a. Why I have defined this particular parameter here, because normally k n would be available in the unit of basis of area; that is per unit area. See now the different area cost. In a normal reaction, without catalyst or other without heterogeneous catalyst, normally we have the rate constant per unit, that is, by multiplied rate by volume in many design in patience.

In the last lecture, I told you that, a solid catalyst reactions or heterogeneous catalyst, the rate is expressed per meter the rate of the catalyst. So, that is why we multiplied by normally to their rate by W, that is, the way to the catalyst right. Now am defining another cost and here which is expressed permit area of the catalyst, which area is a area present in the phoned, can the very large; so per unit area of the catalyst. So, if it is have a rate constant per unit area on the catalyst, it has to be multiplied by the surface area per unit.

So, this gives me k n into S a the rate constant per unit weight of the catalyst, because k m is permanent area, S a is area per unit weight for this becomes per unit made of the catalyst right and row c if I have multiplied by row c, the n it becomes by normal rate cost that is per unit volume of the catalyst. So, this is nothing but the rate constant expressed per unit volume of the catteries. It may be noted that k m in some stander reactioning in the text book like, for a example, of g y m smith, k n is taken to be per unit mass of the catalyst. So, in that case k n that they are using the book equivalent k m into S a there is surface area that you using in locations. I hope it is clear. So, this to gather to all these parameters together is nothing but is normal cost rate per unit volume the cost list. What is the actual rate of the unit of the cost rate?

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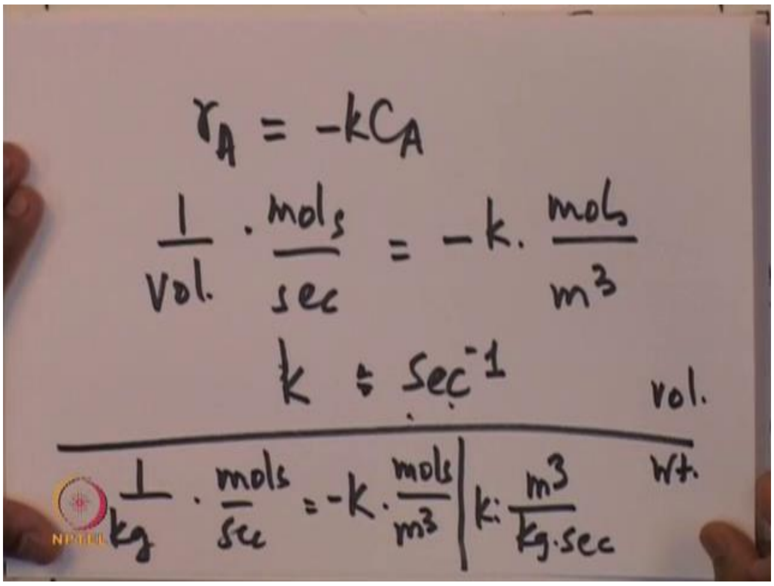

$$r_A = -kC_A$$

$$\frac{1}{Vol.} \cdot \frac{mols}{sec} = -k \cdot \frac{mols}{m^3}$$

$$k \doteq sec^{-1}$$

vol.

$$\frac{1}{kg} \cdot \frac{mols}{sec} = -k \cdot \frac{mols}{m^3} \quad \Bigg| \quad k : \frac{m^3}{kg \cdot sec}$$

Wt.

For a first order reaction r A is equal to minus k C A. And if I want to get unit of r A is expressed; it is a per unit volume of a rate moles per second is equal to minus k molecules per meter cube, what is the reaction which is second minus 1. This is the k normally, this is a per unit volume, because I am expressing rate per volume. But for a first time reaction, unit is second inverse right. That is the unit of first order rate constant when the rate is expressed per unit volume.

Now, if I express rate for a first order reaction per unit weight of catalyst. So, what is the unit hour rate constant? This look at this, now this is for volume per minute volume. Now I would look weight, weight of the catalyst. Now r A is expressed per kg of catalyst, moles per second moles per meter cube right. So, what is the unit of k here?

Unit of k is meter cube per kg second right. This is for volume, this for the per unit weight, this is per unit volume; this is per unit weight right. Now what about the unit when I express where rate per unit area? Area of the catalyst?

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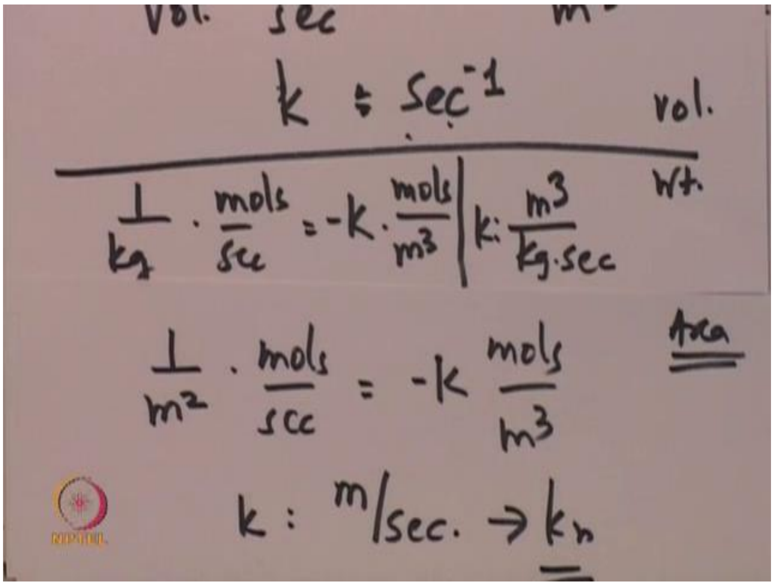

$$k : sec^{-1}$$

vol.

$$\frac{1}{kg} \cdot \frac{mols}{sec} = -k \cdot \frac{mols}{m^3} \quad k : \frac{m^3}{kg \cdot sec}$$

Wt.

$$\frac{1}{m^2} \cdot \frac{mols}{sec} = -k \frac{mols}{m^3}$$

Area

$$k : m/sec. \rightarrow \underline{k_n}$$

1 upon meter square moles per second minus k mules per meter per cube; this is for area, basis is area of catalyst. So, what is the unit of k here? So, unit of k is meter per second and this is nothing but our k n, that we have just we written in our balance along speedical particle, the k n right. So, let me summarize.

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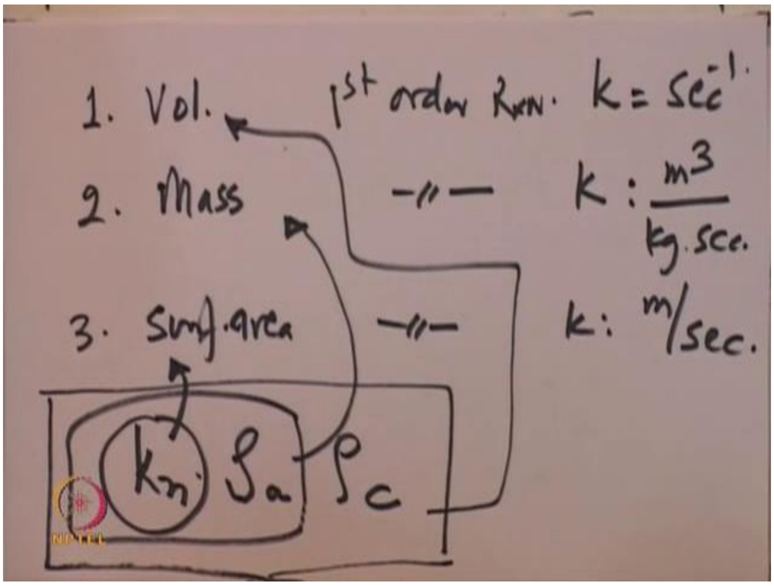

I have 3 type of rate constants expressed per unit volume. For a first order reaction, k has a unit second inverse. Second: unit per mass of the catalyst right, first order reaction k has a unit meter cube per kg second. And third surface area of catalyst, first order reaction k has a unit meter per second. So, these are the 3 different unit that we probably going to deal with as solve the problems later.

So, in our rate equation k n is this right, k n is this, then k n include S a is this and k n into S a into row c that is the density of catalyst particles, then it is nothing but rate constant per unit volume. So, let gets back the equation, the original equation that we have derived. You have this equation. In this, you have entire k n S a row c nothing but rate constant per minute volume. Now why we do all this? We are doing all this to get concentration profile inside a particle. We need to get we need to know how concentration changes has we go from external surface to the interior surface of the catalyst. And why do want all that, because later on I am going to deter min how much is the reduction the concentration and because of which, how much in the reduction in rate, overall rate when diffusion is important. That is the purposes.

Now, we have the differential equation or a need to now the condition first, to solve this differential equation and to get concentration profile inside a catalyst surface all right.

So, what is the boundary here? I have a particle which is second order differential equations. I need 2 boundary conditions.

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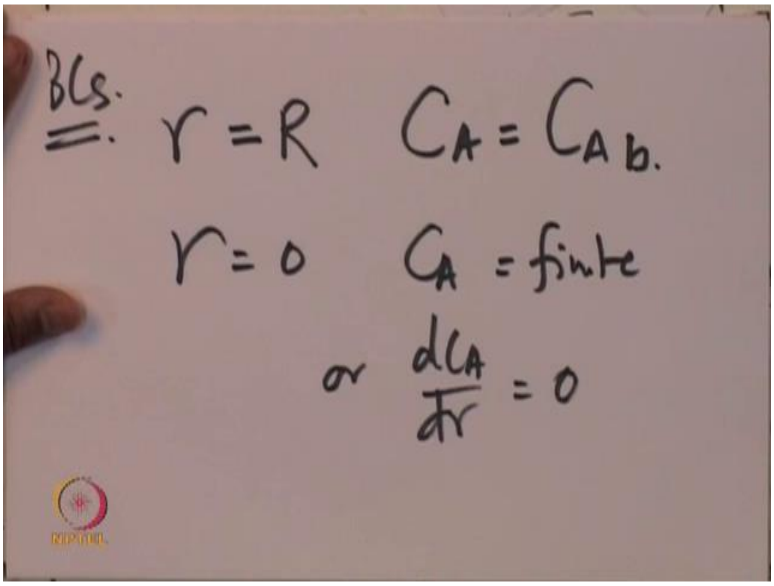

BCs.

$r = R \quad C_A = C_{Ab}.$

$r = 0 \quad C_A = \text{finite}$

or $\frac{dC_A}{dr} = 0$

So, at r is equal to R, I have C A is equal to C A bulk or 0 whatever outside concentration right. Since external effect are not present, we all assuming that C A s equal to C A b which something would I see is and which something would I measure. I cannot go inside a pore and get a concentration or measure a concentration. I see a concentration only in a bulk, why the concentration inside particle is lower than what you have outside, it has to be lower why, because that is a resistance face by the molecules while defusing from a external surface to the interior.

Since, there is a concentration; there is a flow that is a flux the diffusion that is taken place. If this diffusion is significant, then the concentration is significant. Even if you have a very active catalyst present inside, it is not going to see concentration a outside a particle, it is going to see the concentration which is smaller than outside right because of it go down. And our aim is other characterize quantify other these particular resistance and reduction in the range, because of the intra particle diffusion.

So, r is equal to R C A is equal to C A b. And is another condensation that I needs equal to r is equal to 0, you have C A is equal to finite or d C A by d r is equal 0. So, we this to boner is condensation, I need to solve discretion and get the contraction profile. 1 side get the contraction profile, my job would be issuer. I would able to now the local rates at ever point inside the particle and form that again calculate the oral rate, which is going to be the actual rate other and is going to be less than, what it would be, when there is now intra particle diffusion the resistance.

So, I have diffusion and I need to farther modify this, to get some dimension less parameters, which are going to give me some idea about importance diffusion. So, less dimension lies section, the dipping certain dimension less variable.

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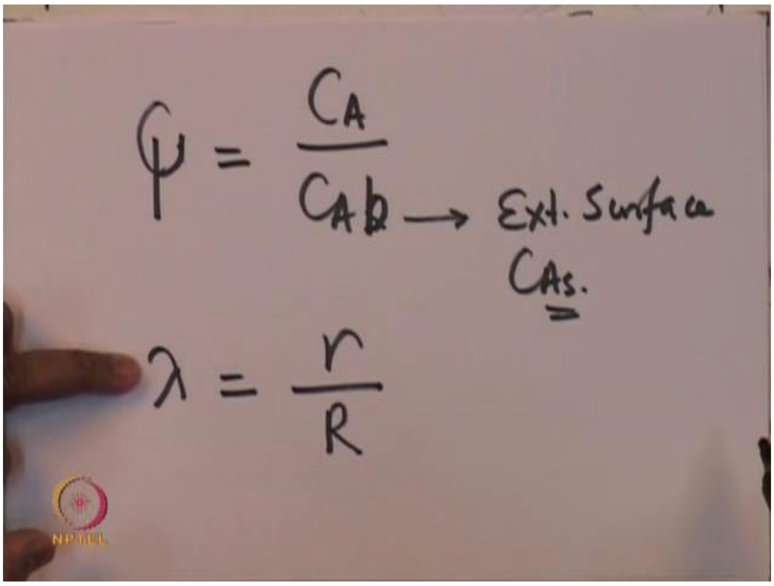

$$\psi = \frac{C_A}{C_{Ab}} \rightarrow \text{Ext. Surface } C_{As}$$

$$\lambda = \frac{r}{R}$$

Let see I have a express contraction as sail equal to C A divided by C A S or C A b other that is what I have use, C A b what is C A b is the bulk condensation is that the external surface, is are the external surface. You can even call this a C A S, some book you may see location C A S. C A b. And then there is another dimension less very able that I defied is; lambda, something do the redial distance r divided by R.

If I have this to variable defied, where dimension less variable, dimension less condensation this dimension less redial distance. If I have that, then my diffusion get radius to a form, this is a diffraction that I have. So, I going to form dimension less concentration and dimension this redial diffusion. What I get this I directly writing this second tried and you whole.

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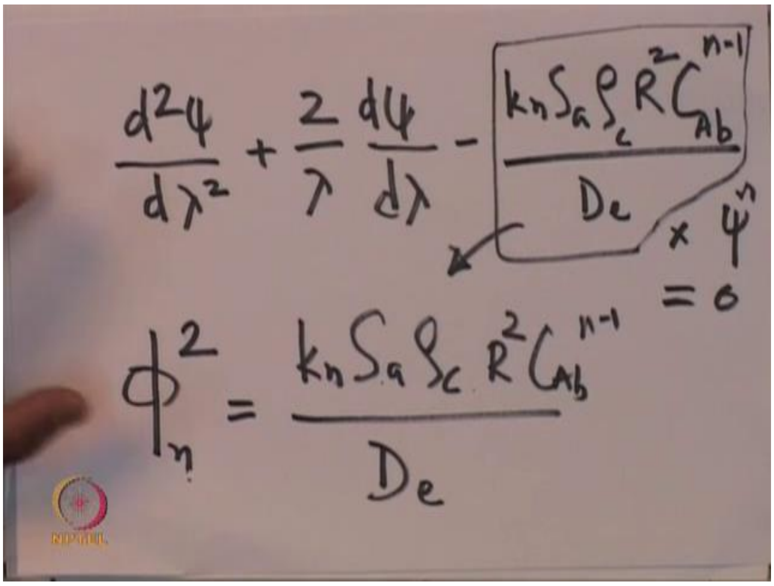

$$\frac{d^2\psi}{d\lambda^2} + \frac{2}{\lambda}\frac{d\psi}{d\lambda} - \boxed{\frac{k_n S_a \rho_c R^2 C_{Ab}^{n-1}}{D_e}} \times \psi^n = 0$$

$$\phi_n^2 = \frac{k_n S_a \rho_c R^2 C_{Ab}^{n-1}}{D_e}$$

So, d 2 sail by d lambda scare plus 2 lambda d sail by d lambda minus k m S a r o c R scare C A b raise 2 n mince 1 divided by D e, that is, diffusivity into sacrifice 2 m equal to 0 So, this becomes by none dimension from of the size dimension less condensation lambda, dimension less redial distance. Now, look at what I got here. This is a term that is going to tell me something. So, let me right that term separately and the no details 5 n..

So, this 5 different from pro city, this not 5 s this 5 n, but they say 5 n square is equal to k n S a row C R. I say square C A b n mince 1 this tram I just writing here aging right. Why square letter to you it makes the situation ease. So, this is the tram. Now, look at the tram carefully, what do you have in this tram. In the nano meter, you have the parameters related to reaction, what you mean; the rate cost, more the rate of reaction is more, surface area ro c. All this parenthetical have something do the reaction. Oppose this R is the expounded for all. This manipulated this execution for the, it is not considered R square and this movement, but otherwise r e c c e the parameters R showing that dependence or there are in the in plans the reaction. What about the denominator D e? D e is something that will affect the diffusion. Now, let me just manipulate this other are other, just play with the situation further.

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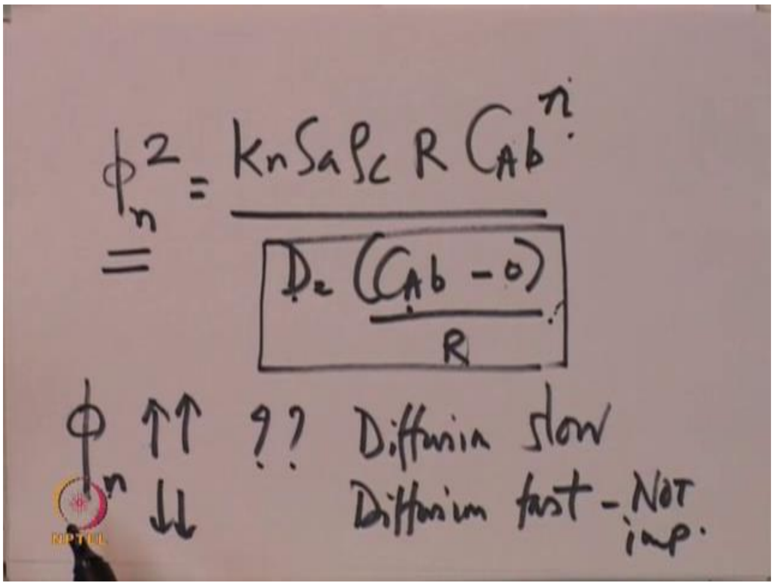

$$\phi_n^2 = \frac{k_n S_a \rho_c R C_{Ab}^n}{\boxed{D_e \frac{(C_{Ab} - 0)}{R}}}$$

$=$

$\phi_n \uparrow\uparrow$?? Diffusion slow

$\downarrow\downarrow$ Diffusion fast - NOT imp.

5 n square is equal to k n S A row c r C A b divided by D e into C A b, C A b n minus 1. Now what I am doing is I am writing C A b n and I taking C A b here minus 0 divided by r. So, what do I see here? I see that this is nothing but the diffusion rate see the condensation ingredient distance diffusivity. Some things, if you have a linear gradient, then this become the flux due to diffusion. Where as a numerator, you have something that will affect the reaction, actual reaction that 2 rates I am comparing here.

So, this partial parameters phi n square is going to give me the relative important of actual reaction, taking place of the site, which may have adsorption desorption surface chemical reaction and all and diffusion. So, relative important of these 2 processes. If phi is very large, what is it mean? It means that diffusion is slow. Diffusion is important. If, phi n is very small, diffusion very fast or not important at all; that means, it like the open catalysts, where no pores the pores is the very large this. So, this value is going to tell me everything.

So, for a given reaction or a given catalysts, if I get the determine the value of phi n or phi n square, the magnitude of this particular parameters, is going to tell me whether reaction important of diffusion is important. If this value is very large, then diffusion is important, important size slow and it is going to control the rate. And if is very small, then I do not need to worry about it, I just take it has if like this no diffusion problem.

So, this 5 n is called us Thiele modulus. It is the very important term a heterogeneous catalysis that tells you the importance of pore diffusion. This term is called as or this particular number is called us Thiele modulus.

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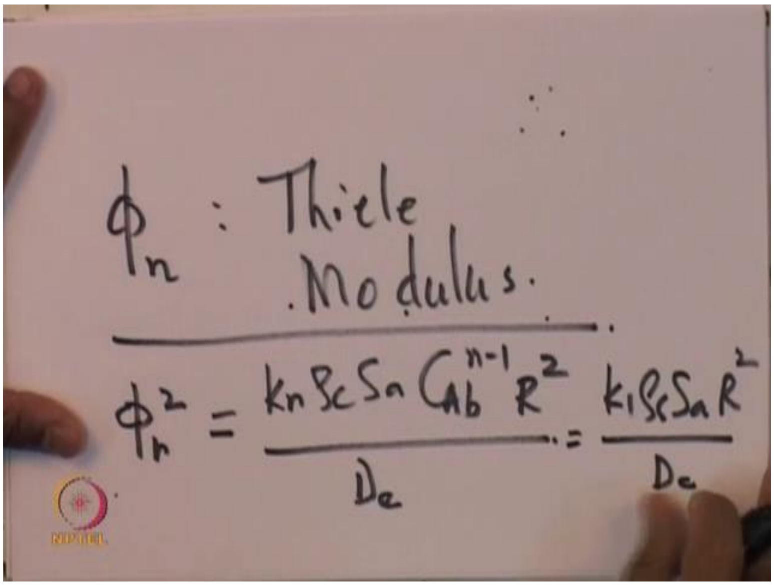

ϕ_n : Thiele Modulus.

$$\phi_n^2 = \frac{k_n \rho_c S_a C_{Ab}^{n-1} R^2}{D_e} = \frac{k_1 \rho_c S_a R^2}{D_e}$$

So, phi m is Thiele modulus. Again write it for different types of reactions; first order the reaction, second order the reaction and so on. So, the equation that I have is for a spherical partial, because I am talking in terms of the radius the partial. If I have cylinder, if I have something else some other shape. So, I have the corresponding characteristic dimension, that is, particular shape. Will look at that separately, like suppose I have a cylindrical pore, how do I write and a expression for how do a derived expression for Thiele modulus.

But right now, I am doing it for a spherical particle and I have the expression given by this that is, 5 n is equal to k m row c S a C A b n raise to n minus 1 R square divided by

D e all right. And suppose n is equal to 1 the first order reaction, because very issue k 1 row c S A R square divided by D e, this is ph n square.

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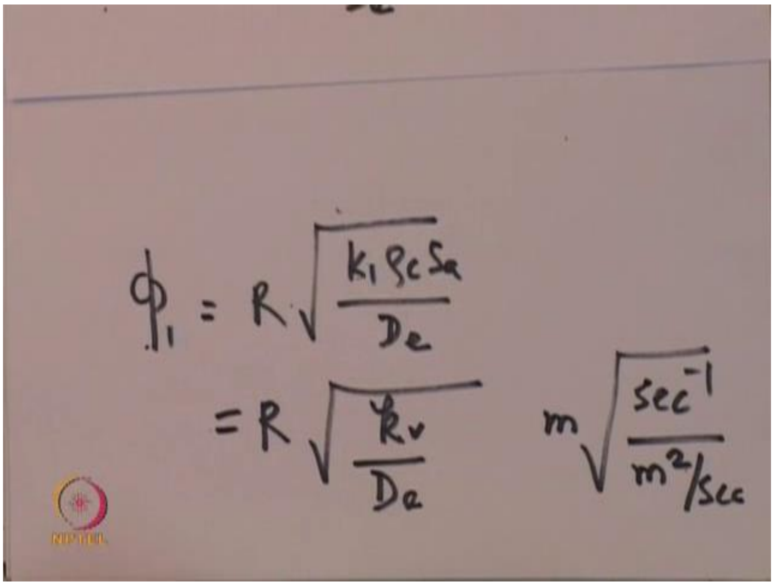

$$\phi_1 = R\sqrt{\frac{k_1 \rho_c S_a}{D_e}}$$

$$= R\sqrt{\frac{k_v}{D_e}} \qquad m\sqrt{\frac{sec^{-1}}{m^2/sec}}$$

Now, phi 1 would be R root of k 1 row c S A divided by D e. If I give rate cost and per rate volume, I do not need to write all this. It would be r k v D e, why k v, because it is expressed in terms of into volume, because this has a unit per unit volume right, first on the reaction, it will be second inverse. This is dimension less number; look at the units R meter k second inverse D e meter square per second. So, if you look at this no units. So, this is the dimension this number, everything will get cancelled all right.

So, remember phi is a dimension, this number called as Thiele modulus, which gives the importance of, tells you the importance of pore diffusion effects. If the value of phi is large, then the pore diffusion effects are significant, I cannot ignore them. And if the value of phi is relatively small, say 0.01 or whatever, then I can safely ignore pore diffusion and treat the reaction as if, there are no pore diffusion effect and the reactions taking place on the catalytic surface which is wide open for me. We will go further and try and simplify this and understand pore diffusion effect, in details. Get some more inside, in next lecture.

Thanks.