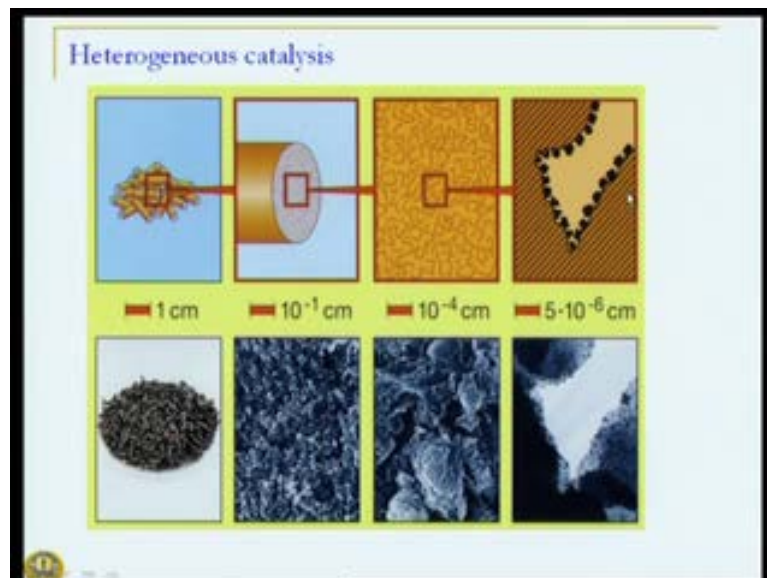


**Chemical Reaction Engineering**  
**Prof. Jayant Modak**  
**Department of Chemical Engineering**  
**Indian Institute of Science, Bangalore**

**Lecture No. # 19**  
**Gas-solid Catalytic Reactions Transport in Catalyst Pellet**

Friends, let us continue our discussion on diffusion and reaction in a solid catalytic particle and to recap, let us look at what is this catalyst particle look like.

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So, if you look at these schematic as well as the asylum photo graphs over here. You will see that this catalyst pellet is made up of pores, but these pores are obviously not straight line pores, there is a tortuous path that reactants have to have to follow. That is one thing that we should keep in mind and also you can see that more clearly in this cartoon, where it says that you have to follow a tortuous path. It is not from one end of the catalyst pellet to another end. There is a through and through a single parallel pore. So, that is one aspect.

The second aspect is about the size of these pores. Now, if you look at this pore, we are talking about micron size pores or at times you could have pores which are even smaller than this. So, typical size of a pore may be anything from 10 angstrom to 10 thousand

angstroms. When it comes to diffusion some other considerations come into picture, because the size of the pore is very small and we will talk about it shortly.

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**Characterization of catalyst pellet**

$100-500 \text{ m}^2/\text{g}$

$S_g$  surface area / gm catalyst

$V_g$  void volume / gm catalyst

$\rho_p$  gm catalyst / pellet volume

$\epsilon_p$  void fraction

$f(r)dr$  void volume distribution

$$\epsilon_p = \frac{m_p V_g}{m_p V_g + \frac{m_p}{\rho_s}}$$

$$V_g = \frac{V_p}{\rho_p}$$

Figure 1.1.1 Pore size distribution of catalyst pellets

So, how do we actually then characterize the pore. There are several quantities of interest, which help us characterizing the pore. What we are essentially talking about. Is this is, let us say my catalyst pellet and through this pellet, are these pores which are randomly distributed and networked and so on and so forth. And it is this inside of the pore onto which my active material is placed. So, is that inside area that is what is of importance to me and sometime back I said, that to the extent that this external surface area is of little relevance as far as the catalytic reaction is concern.

We characterize the catalyst for example, using surface area per gram of catalyst  $S_g$ . So, that is all these area that **all these area that** we that is available inside the catalyst pore per area. And mind you this value can be significantly high. it can be as high as 100 to 105 meter square per gram surface area. That is one quantity of interest.

The second quantity of interest is, as you will realize that this particle which we have shown as spherical particle is not all solid blocks. So, it consist of voids through which the gas will flow and the solid material. So, we have voids and then we have the solid material. The catalyst actually consists of both these things. So the quantity of interest

therefore is not the total volume of this catalyst pellet, because if it is a solid block total volume has no meaning, because there is no space for gas to flow. What is of importance is the void volume. We have void volume  $V_g$ , which is all this volume that is available for material or gases to flow through per gram of catalyst.

Then we have another quantity of interest  $\rho_P$  that is the density of the density of the catalyst pellet,  $P$  stands for pellet here. And it is important to distinguish it from the density of the solid material which makes the catalyst. For example, if we say that the density of the solid material is  $\rho_S$ , then we will have density of the catalyst. How does it work? Density of the solid is, let us say  $\rho_S$ . The density of the catalyst pellet, so when we are talking about pellet volume, pellet volume here consist of both void volume and the solid volume. That is actually put together is the pellet **pellet** volume and hence the effective density of the catalyst pellet  $\rho_P$  is different than the density of the solid material which makes the catalyst **catalyst** pellet.

We then have another important property  $\rho_P$  or rather  $\epsilon_P$  which is the void fraction. And void fraction is nothing but the volume of the void divided by the volume of the catalyst **catalyst** pellet. So, these quantities of course are not completely unrelated to each other. So for example, we could write  $\epsilon_P$  as mass of the catalyst pellet  $m_P$  times the density the void volume. Gram of catalyst into the void volume  $V_g$ , so that is the total void volume divided by, let me remove this catalyst, so  $V_p$  divided by void volume plus the mass divided by the density of the solid. This is the volume occupied by the solid and this is the volume occupied by **this is the volume occupied by** the voids, this is the volume occupied by solid. Ratio of these two quantities is nothing but my void fraction. If you rearrange these terms, we will actually get **we will actually get** my  $V_g$  is  $\epsilon_P$  by  $\rho_P$   **$\epsilon_P$  by  $\rho_P$** . These quantities are actually related to each other they are not completely independent of each other.

Another quantity which is of interest when we characterize the pellet is what is the distribution of this void volume? That is, if we look at look at this cartoon, the radius of all this catalyst pores is not same. So, in other words whatever is the void volume there it is not of the same size. So, there is a distribution of this void age and this is also important quantity. And for example, in a typical catalyst, you will find there are ways of measuring these void **void** volumes by penetration method, that is you force mercury to

penetrate to the catalyst pellet. And the force required or the pressure required is inversely proportional to the size of the catalyst pore. And from that one can get a distribution, the first example on the top here. On the x axis is our radius in angstroms and this is the volume fraction or void fraction.

It is a typical Gaussian distribution, which says that the average size would be somewhere around this particular value over here and roughly, let us say 20 or 30 to 40 angstroms, but there is a distribution.

So, there are pores which are as big as about thousand angstroms, but their fraction is small. There are pores which are as small as 10 angstroms, but that fraction is also small; majority of them is in this range. But one could also have depending on how the catalyst is made, a bimodal distribution. For example, in the second case again same radius on the x axis, the void fraction on the y axis. we see that there are two peaks actually. There are pores which are about 1000 angstroms in a micron range and there are pores which are about 20 to 30 angstroms.

So, this is a bimodal distribution. So, we have macro pores and we have micro pores. So that is also possibility. This is how we typically characterize the catalyst pore.

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The slide is titled "Transport in pore" and illustrates three flow regimes: Bulk, Knudson, and Viscous. Each regime is represented by a diagram of a pore with arrows indicating the dominant transport mechanism. Below the diagrams is the general equation for the molar flux  $N_j$ :

$$-\frac{1}{RT} \nabla p_j = \sum_{k \neq j} \frac{1}{D_{jk}} (y_k N_j - y_j N_k) + \frac{N_j}{D_K} + \frac{y_j}{D_K} \left( \frac{PB_0}{RT\mu} \right) \nabla P$$

Below this equation is the equation for Knudsen diffusion coefficient  $D_K$ :

$$D_K = \frac{2}{3} \bar{v} \left( \frac{8RT}{\pi M_j} \right)^{1/2}$$

Handwritten notes in blue ink specify  $\bar{v} \approx 10^{-50} \text{ m}^3$  and  $1 \text{ atm } l \approx 1000$ . A lecturer is visible in the bottom right corner of the slide frame.

Now, before we turn our attention to chemical reaction and look at what happens when the reaction takes place? Let us look at once again the transport in the pore. Now, when it comes to transport in the pore, there are three different ways in which gas can flow through the pore. For example, bulk diffusion. Now, bulk diffusion arises because of molecule to molecule contact.

Now in a reactor, for example, whose dimensions are in meters, this is a dominant phenomena of diffusion bulk diffusion. However when it comes to pore, because the size of a pore is small, there are several other ways which also drive the reactant through the pore.

For example, the first one that you see over here is a case of bulk diffusion. And this is a common phenomenon, if we look at the bulk that is it is same as whether it is flowing in a reactor or flowing in a pore. And what we what equation which is shown over here, is actually calculating the total gradient or driving force for the material to flow. It has first component, which is the bulk flow. So, this component represents the bulk flow. So, the flow is due to molecule to molecule contact, but it turns out that, if your pore size, for example of the order of 10 angstroms or 1050 angstroms of that order. Then the likelihood that one gaseous molecule will interact or hit the other gaseous molecule, So molecule to molecule contact is much smaller than the gaseous molecule heating the wall of the pore.

And this phenomena, and therefore diffusion which is driven because of contact between the gaseous molecule and the wall of the pore is refer to as Knudsen diffusion. And the second term that we see over here is a contribution of Knudsen diffusion. That is primarily because of contact between molecule and gas.

Now, how does this come about? Typically, if you consider a gas at one atmosphere **So one atmosphere**, the mean free path  $l$ , as it is known as that is the distance on an average a gas molecule has to travel, before it can heat another gas molecule, is of the order of 1000 angstroms.

So, if your pore size is in access of that, let say 1000 micron, then before the there is a good chance that molecule to molecule contact will take place and diffusion can happen.

But what about, if the size is only 10 angstrom? So, molecule has to travel about 1000 angstroms to heat another molecule, but before it can do that, it will heat the wall, because the wall size itself is 10 angstroms and hence this what we call Knudsen diffusion. And the Knudsen diffusion is characterized by Knudsen diffusion coefficient, which is given by this formula over here. And this tells us that it depends on the size of the pore  $R$  bar depends on the temperature and depends on the molecular weight of the species. Notice here, we represent Knudsen diffusion as  $d_{k,j}$  for Knudsen and  $j$  for the species. And it is tied down to the property of the species  $m_j$ , but notice here that it does not involve another gaseous molecule. Whether it is a multi component system or a binary system or whatever may be the system the diffusion is independent of what is what else is there. That is a characteristic of Knudsen diffusion.

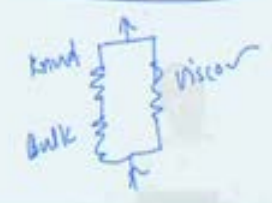
The third phenomena in by which material can flow particularly when we are looking at capillaries and pores, as capillaries, is that from inlet to the outlet there will be significant pressure drop. And this pressure drop will drive the flow of material through the pore. This is referred to as viscous force. And using darcy's law this can be represented as the pressure driven force through the catalyst **catalyst** pellet. We have three different three different phenomena which drive material through the catalyst pore bulk diffusion, Knudsen diffusion and viscous force.

This is just like a flow through a tube, but in this case the tube is of 10 angstrom or 100 angstrom. So, pressure drop can be significant.

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Transport in pore

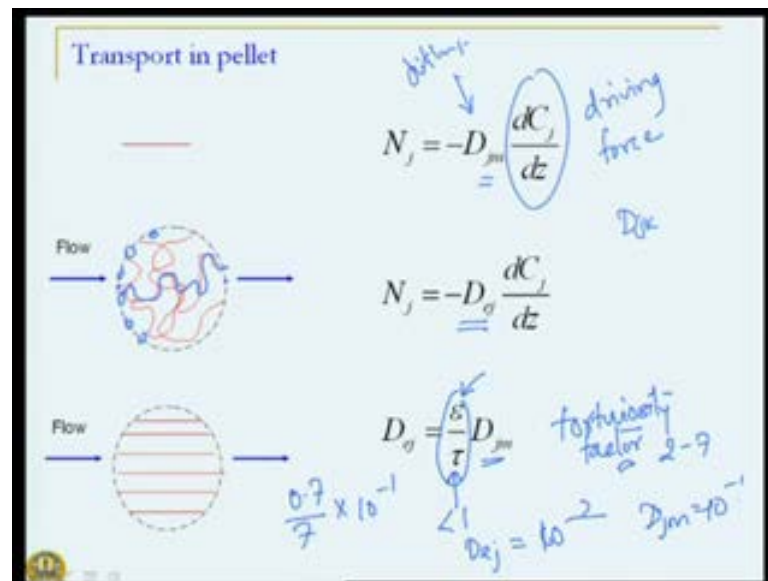
Bulk Knudsen Viscous

$$-\frac{1}{RT} \nabla p_j = \sum_{k \neq j} \frac{1}{D_{jk}} (y_k N_j - y_j N_k) + \frac{N_j}{D_{Kj}} + \frac{y_j}{D_{Kj}} \left( \frac{PB_0}{RT\mu} \right) \nabla P$$
$$D_{Kj} = \frac{2}{3} \bar{v} \left( \frac{8RT}{\pi M_j} \right)^{1/2}$$


And hence this term which involves pressure drop driven. What you see here **what you see here** as a model of entire diffusion is what is referred to as Mason Andean's dusty gas model, which assumed Knudsen and bulk diffusion in series. So, the actual model used is analogy with an electrical circuit.

This is your Knudsen diffusion, this is your bulk diffusion and this is your viscous force and this is the flow. If you take that that model, finally we end up with this kind of representation. The point I am trying to making here is, therefore that there are various different factors which contribute to the diffusion.

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This is not the end of the story, because as you can see here we have represented this catalyst as a single pore. But catalyst, of course is not a single pore. It is a pore, catalyst actually is a combination of different sizes of pores, different orientations of pores and so on.

if we once again revisit the diffusion phenomena, this is how diffusion phenomena is influenced when you consider transport in the pellet. For example, if you just consider bulk motion, **bulk motion** we can write the flux  $N_j$  as minus  $D_j \frac{dC_j}{dz}$  that is this is the driving force and this is the diffusion coefficient. Notice here, we use  $D_j$ , because we do not have binary components always. We do not have diffusion coefficient  $D_{kj}$  and  $K$  is 2 elements, but we saw earlier there is a relationship and equivalent effective diffusion is defined in a mixture,  $j$  in a mixture.

However, there are two complications that arise. One, if you look at the flow direction, normal to the flow direction not the entire surface is porous. So, there are pores, some solid, and some pore volume. If you want to define the flux in terms of what is happening, which of is the flow we have to define the flux, see this is a diffusion coefficient, these diffusion coefficient gets modify and these becomes effective diffusion **effective diffusion** coefficients. Difference between this two is, this we are assuming a multi component mixture in bulk process, bulk diffusion.



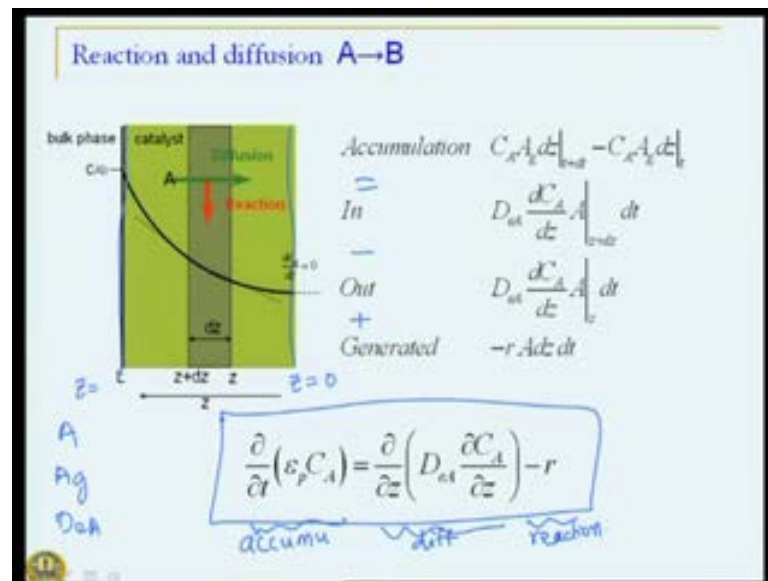
Here, effective diffusion, because of two different phenomena. Number one, if you look at the cross section which is now exposed to this flow over here not entire surface is available for flow. So, there are these void volumes through which only this material can flow. If you talk in terms of the area available for flow, it is not the entire area, but the void area. So, diffusion coefficients, if you are going to describe the flux in terms of properties of the catalyst pellet, surface area let us say, this  $D_j m$  from here has to be modified, because only a fraction of this is available for flow. And that fraction can be the void fraction.  $D_j m$  gets multiplied by the void fraction.

Another modification has to be made, because the direction of the flow that is this x axis as shown over here is not the actual direction of flow inside the catalyst pellet. For example, inside the catalyst pellet, the material may flow changing directions several times or in other words, the path that gaseous reactant molecule actually travels is much more than the path as represented by these x axis, that is from this end to this end. The diffusion rate therefore decreases, because it has to now travel a longer path. And if you are again describing the flux in terms of the major flow direction or the flow direction of the bulk, then we have to introduce another factor now which is called tortuosity factor, which is anywhere from 2 to 7 roughly greater than 1.

what it means is that the actual effective diffusion coefficient is lower compared to the bulk diffusion coefficient, because of two things epsilon, void fraction which is less than unity and tortuosity factor, which is greater than one. Both these will contribute to this fraction being less than one. And therefore, the actual diffusion coefficient is something less.

For example, to give you just an idea, suppose  $10^{-1}$  was  $D_j m$   $10^{-1}$  was  $D_j m$  epsilon was 0.7 and tortuosity factor was 7, then the actual effective coefficient  $D_j$  would be  $10^{-2}$  whereas, the bulk diffusion coefficient is  $10^{-1}$ , almost an order of magnitude lower. This is just a sample example.

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So, now having got some idea about how the material is moving through this catalyst pellet. Let us now turn our attention, actually to reaction and diffusion. What we are now going to do is look at a mass balance, which is applicable when material is both diffusing and reacting.

What we are going to do is we are going to consider only as lab geometry to begin with. Essentially, what we are looking at is as lab geometry. We will start our discussion with first order kinetics and isothermal situation. This will be our base or starting point for analyzing diffusion and reaction. Little later on, we will relax all these restrictions. We will see what happens when your geometry is spherical or cylindrical or for that matter an irregular geometry. We will see what happens when the reaction is not first order reaction, but general power law kinetics or law of mass action kinetics or (O) kinetics which we saw earlier. And we will also see what happens, if the reaction is accompanied by either release of energy, exothermic reaction or absorption of energy, endothermic reaction. So, essentially non isothermal case.

When these effects are strong, what happens? But to begin with, let us consider slab geometry. So, what we have here **what we have here** is a catalyst of this size **catalyst of this size** this is the half width, recall our discussion wise catalyst as symmetry. So, we are looking at only half. So, center is my Z equal to 0, Z equal to 1. So, half width is 1, on this side is a bulk phase and the concentration is  $C_A$  of my reactant my reaction is a going

to  $b$ . and we are going to assume that our catalytic material is uniformly distributed through end these entire catalyst **catalyst** pellet. These entire catalyst pellet and therefore, we are now going to setup the mass balance.  $Z$  is my actual coordinate. So, I will look at what is happening between location  $Z$  and  $Z + dZ$ . What is happening **during this** during this small cross section?

We will set up a mass balance on this on this cross section. This is the outer surface and this is the centre. Now, we can we have seen these earlier, what will typically happen, is gas will flow in. we are not considering external resistance as of now, but we will bring that in little later on, something which we discussed at the beginning of this session on heterogeneous catalysts.

The concentration at this point is the bulk concentration  $C_A^b$  and concentration will decrease gradually, as material moves through this porous catalyst. What is responsible for moment of this material, there is diffusion, but along with diffusion there is a reaction also. So, we will have to account for all these processes.

Let us define few terms, for example, we our area cross sectional area that is area perpendicular to the flow is let us say  $A$ . Of this  $A$  only  $A_g$  is available for material to flow, because that is a void or gaseous volume void volume. Then diffusivity, we now understand we are going to say  $D_{eA}$  effective diffusivity. So, we have accounted for all tortuous paths and so on and so forth.

Let us write down the mass balance. For a short time duration  $T + \Delta t$ , concentration multiplied by the volume  $A_g \Delta z$ ,  $A_g \Delta z$  is the void volume now. concentration also defined as moles per void volume. So, this is the mass which is present at time  $t + \Delta t$  and the same quantity  $C_A A_g \Delta z$  at time  $t$  that is present at time  $t$ , the difference between the two tells me, how much mass has accumulated in this cross section, small section of this catalyst pellet.

This accumulation is a result of material coming in. it is coming in at  $Z + \Delta z$  **it is coming in at  $Z + \Delta z$** , because of diffusion. So, the flux that is moles per unit area is given by  $D_{eA} \frac{dC_A}{dz}$  multiplied by the area  $A$ . Remember while defining effective diffusivity, we incorporated per unit area cross sectional area, not the void area that is why we multiplied our  $D_{jm}$  by  $\epsilon$ . So, that multiplies by  $\epsilon$ . This is the moles that

are coming in at  $D_z$  or molar rate rather flux rate and in time  $D_t$ . This is how much has come in, the same quantity evaluated at  $Z$  is what is going out **what is going out** and what is generated in this element. If  $R$  is the rate of these reaction then and we are looking at species A, which is actually getting consume.

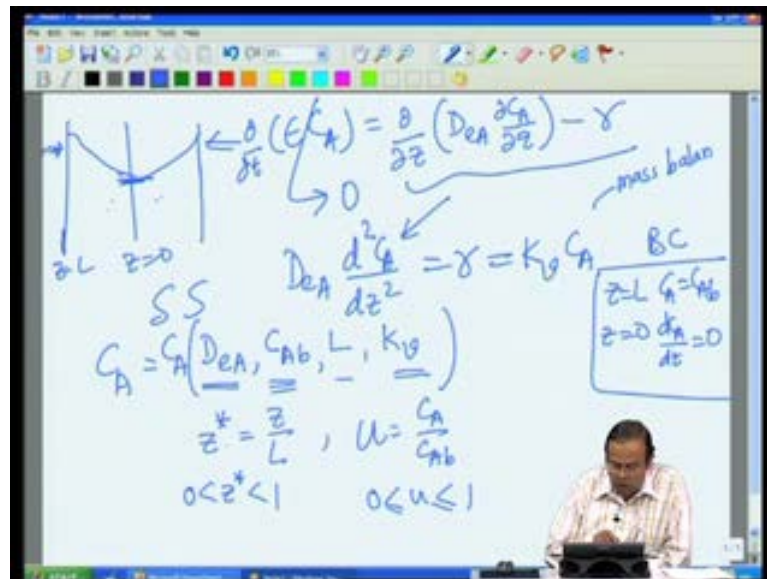
Stoichiometric coefficient  $\nu_A$ 's  $R$  will be the rate of generation. In this case stoichiometric coefficient is minus 1. So, minus  $R$  is the rate of generation or in other words  $R$  is the rate of consumption. We just make it minus  $R$  for making it in a normal form. this is per unit volume of the catalyst pellet, let us say multiplied by the volume of the catalyst pellet  $V_p$  into  $D_z$ , that is the moles of A which are generated or rather rate at which moles of A are getting generated multiplied by small  $d t$  that is the time interval which we are looking at. So, our mass balance is fairly straight forward.

Accumulation is equal to in minus out plus generation. Putting corresponding terms dividing by a  $D_z D_t$  taking limits as  $D_z$  goes to 0,  $D_t$  goes to 0, we get the overall mass balance equation or unsteady state diffusion reaction equation.

This quantity representing accumulation, this quantity representing diffusion and this quantity representing reaction. We have mathematical model of diffusion or a diffusion reaction equation, unsteady state equation. What kind of equation is it? Is a partial differential equation time and actual position  $Z$  involves void volume, concentrations, diffusion coefficient and rate of reaction.

Let us let us look at these equations, but let us look at the solution of these equations, but let us play little bit with these equation.

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So that, before we move onto looking at the actual results. What we have here, is the differential equation of the concentration of A. The first simplification, that we are describing a slab from  $z=0$  to  $z=L$  over here.

What we are going to do? We are first going to make an assumption that as far as this process is concerned that is just steady state. So, this term goes to 0. We have a steady state balance and partial differential equation, now we will convert into ordinary second order differential equation. And we will also assume that  $D_{eA}$  is constant.

So, we will get from this equation steady state version. This is my steady state mass balance equation for diffusion reaction. This diffusion reaction equation incidentally has been used in variety of different ways not only for catalysts, but for describing diffusion through tissues of our body, diffusion through lung, diffusion through plants. You talk about any process which involves diffusion invariably there is a reaction, I mean not all, but majority lungs. For example, oxygen is taken in or diffuses is released to the various organs. It is kind of a **kind of a** reaction situation.

We have variety of different use for this. Now at this point, let us bring in that the reaction is first order. Mind you, this balance that we wrote we don't make any

assumption on kinetics. That is a general mass balance for slab geometry, but let us make an assumption that this is a first order reaction. This is the first order reaction. The second order equation, mathematically speaking we need two boundary conditions and these two boundary conditions are provided by at  $z$  equal to  $l$  at  $Z$  equal to  $l$  at this interface my concentration is the bulk concentration.

And if you recall, we have symmetry the gradient at this particular point is 0. So, that condition can also be written as what it means is that, if you have an if you have a catalyst which is exposed to the gaseous reactant from all sides. Then at the center point material can, if it is a symmetric case material cannot flow from one region to another. They cannot be cross over, because material is suppose this is our full catalyst material is coming in from here from here. So, there cannot be any diffusion across this center point. Because if there is diffusion from here this side to this side, there will be a counter force to drive material from this side to this side, net result is no diffusion across this center point.

Or in other words the flux at the center is 0. So, that gives me my second boundary condition. That is at  $z$  equal to 0 flux is 0. These are my two boundary conditions, which I will use for solving this equation. So, let me write down those boundary conditions on the side,  $Z$  equal to  $l$ ,  $C_A$  equal to  $C_{A,b}$ , and  $Z$  equal to 0, this flux equal to 0 can also be written as  $D C_A / D z$  equal to 0. So, these are my boundary conditions, this is my mass balance steady state.

Now, we would like to look at how this solution looks like. And to see that let us try to before we look at the solution with these boundary conditions, let us try to manipulate these equation little bit, before we see these solution. The reason for manipulation will become clear in a minute.

Now, if you look at these mass balance equations, there are four parameters diffusion coefficient, concentration of bulk  $C_{A,b}$ ,  $l$  that is characteristic of the pellet and then there is  $K_V$ . This diffusion mass balance along with its boundary condition involves four different set of parameters.

This is a characteristic of the pellet that is the material, this also in some sense is a

characteristic of a pellet, this is the characteristic of the reaction and this is also part of reaction that is what the bulk concentration that is present is. If we now solve these equation as it is. You can expect the concentration  $A$  as a function of these values. There is it will depend on these values of these four parameters.

So, anytime you change one of the parameters, the other the entire solution will change. But rather than doing this, there is an elegant way of solving these equations by making the equation dimensionless. Let us try to make this equation dimensionless. By saying that I am going to define my actual co-ordinate in it  $z$  star as  $z$  by  $l$ . So,  $z$  star can go only from 0 to 1. and I am going to call my concentration  $C_A$  star or rather let me call it as  $u$  that is a standard notation  $u$  as  $C_A$  by  $C_{A,b}$ . What I have essentially done by doing this kind of dimensional exercise, I have converted my concentration term into dimensional less concentration  $u$  with  $u$  between 0 and 1.

Similarly, I have converted my actual coordinate  $Z$  instead of in microns or angstroms or whatever you units that you want to put it. This also is between 0 and 1. My one idea of making this equation dimensionless is that all the order of magnitudes of both these variables is now between 0 and 1. So, when you solve a numerical equation, if that order of magnitude of various terms differs then you sometimes land up in numerical difficulties. This is one way of making sure that numerical difficulties are avoided, because order of magnitudes of different terms is different.

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The image shows a whiteboard with handwritten mathematical derivations. At the top, the differential equation is written as  $\frac{d^2 u}{dz^2} = \left( \frac{L^2 k_v}{D_{Ae}} \right) u = \phi^2 u$ . Below this, the Thiele modulus is defined as  $\phi^2 = \frac{L^2 k_v}{D_{Ae}}$ . This is further simplified to  $\phi^2 = \frac{L^2 / D_{Ae}}{1/k_v}$ , with units  $m^2/m^2/sec$  shown. The term  $1/k_v$  is identified as  $t_{\text{reaction}}$ , and  $L^2 / D_{Ae}$  is identified as  $t_{\text{diffusion}}$ . The final simplified form is  $\phi^2 = \frac{t_{\text{diffusion}}}{t_{\text{reaction}}}$ . A note states that the Thiele Modulus  $\phi$  is very large when  $t_{\text{diffusion}} \gg t_{\text{reaction}}$ .

Now, if you substitute all these **if you substitute** these Z star and u into our mass balance equations. We actually get our mass balance equation in the following form; d square u by d z star square is equal to L square K V divided by D A e into u. So now, if we **if we look at** look at this **look at this** term look at the term l square K V by D A e. What are the dimensions of this term? Without even checking the dimension of each of this term, we can clearly see the left hand side is dimensionless d square u by z square. So, right hand side also must be dimensionless, u is already dimensionless. So, this term must be a dimensionless quantity.

And indeed it is a dimensionless quantity and we call these as Thiele modulus phi and it is represented as phi square. Where Thiele modulus phi square is defined as L square k v by D A e. Now, what is the advantage now? So, our equation is now in a dimensionless form, but more than that. If you look at this equation which we actually derived from this equation this mass balance. Dimensionless form of our reaction equation compared with the same, but dimensional form this had four parameters D A e, C a b, l, K v this has only one parameter phi square.

By making equations in a dimensionless form, we have actually compress the parameter range or space into from 4 to 1. And now you can see a clear advantage that if I have, let me write my phi square over here. So, my phi square is L square K v D A e, let us say its



value is 1. If phi square value is **phi square value is** 1 irrespective of what combination of  $L$ ,  $K$ ,  $v$  and  $D$ ,  $A$ ,  $e$  gave me this value 1, my solution in terms of dimensionless quantities will be identical. Various different values of  $L$ ,  $K$ ,  $v$  and  $D$ ,  $A$ ,  $e$ , all of which result into phi square value being equal to 1, has a same solution in terms of dimensionless quantity. of course in terms of dimensional quantities the solutions will differ. But all are therefore need, is to solve these equation  $u$ . So,  $u$  is now only function of phi. Instead of  $C$ ,  $A$  being functions of this four variable. If I solve it for one value of phi, I have actually solved for several different values of these four parameters those we that we have.

What does this Thiele modulus represent? **what does this Thiele modulus represent?** Now, if we look at these Thiele modulus, phi square which is  $L^2 K V$  by  $D A e$  which I can also write as  $L^2$  by  $D A e$  divided by  $1$  by  $K V$ . This is the small algebraic manipulation. What are units of  $L^2$  by  $D A e$ ,  $L$  is in let us say length scale. So, length scale square divided by  $D A e$ . Let us take typical units. So, this is  $m^2$  for length and this is let us saying  $m^2$  per second. So, what are the units of these? Units of these are in seconds the numerator denominator also must be in seconds. These have numerator both numerator and denominator has time units. So, what time is this? Now, if you look at the denominator first,  $K V$  is the reaction rate constant which has a unit of time inverse.  $1$  over  $K V$  is actually the characteristic time of reaction **characteristic time of reaction**. Which will tell us, how fast what are the time scales on which the reaction is taking place?

By same analogy,  $L^2$  by  $D A e$ ,  $L$  is the actually the diffusion length. Therefore time characteristic time for diffusion. What does it mean? It means that our Thiele modulus is actually comparing two different phenomena, diffusion and reaction. And that is natural, because these are the two phenomena occurring diffusion with chemical reaction. Thiele modulus is actually the ratio of diffusion time to reaction time.

Now, we can qualitatively characterize reactions as follows. For example, if phi is very large and what is that very large? We will see it in the next session, but if phi is very large, what it means? It means the characteristic diffusion time is very much in larger value than the reaction time. That means, the time scale on which diffusion is occurring is much larger than time scale on which reaction is occurring. Other way of putting that would be diffusion is a slow phenomena compared to reaction.

So,  $\phi$  value very large would imply that diffusion is a controlling behavior. Remembers our idea that whosoever slow controls. Here, if  $t$  characteristic time for diffusion is much larger than characteristic time for reaction, diffusion is a slower process. So, diffusion must be controlling. On the other hand, if  $\phi$  value is very small or Thiele modulus is very small, diffusion time scales are much shorter than the reaction time scales.

That means reaction is very slow. We can therefore, see two extreme or limiting cases Thiele modulus very large diffusion controlled process, Thiele modulus very small reaction control process. With this, we will stop for today. And in the next session, we will look at how this concentration the diffusion reaction equation, how does the solution look like. And what do we get out of all this exercise. What are the actual reactions rates that catalyst particle will follow or the reaction will follow. **thank you**