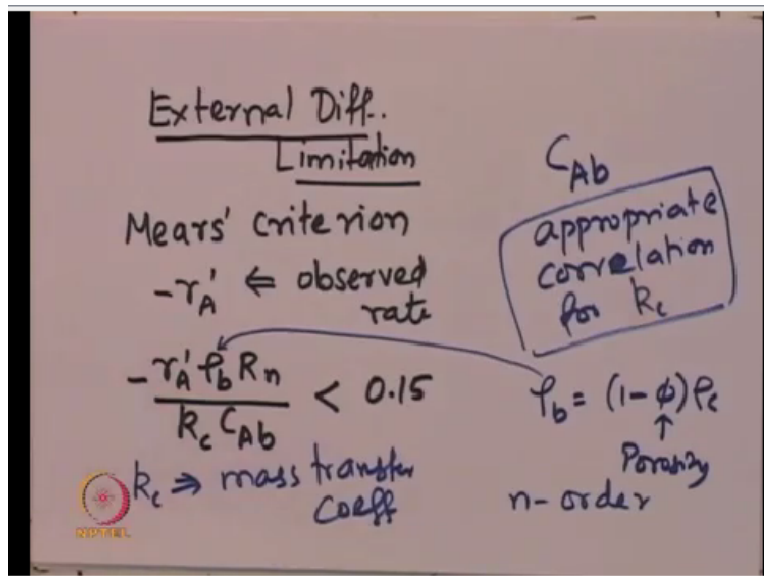


Chemical Reaction Engineering - II
Prof. Ganesh A Viswanathan
Department of Chemical Engineering
Indian Institute of Technology - Bombay

Lecture – 34
Packed - Bed Reactor Design

Now let us move on to the external diffusion. We looked at the internal diffusion. What is the method to use the experimental observable data in order to find out whether the reaction is being conducted under internal diffusional limitations? So next let us look at the external diffusional limitations.

(Refer Slide Time: 00:49)



So one has to use a criteria developed by Mears, it is called the Mears' criterion. So Mears' criterion can be used to find out whether the catalytic reaction is being conducted under external diffusional limitations, that is mass transport diffusional limitations is the transport of species from the bulk to the surface of the catalyst is that limiting the reactions severely. So the expression is suppose if $-r_A$ is the observed reaction rate, is the observed rate, then the criterion is that if $-r_A \cdot \rho_b \cdot R^n / k_c \cdot C_{Ab}$, if that is smaller than 0.15.

So if the ratio of, if this expression on the left hand side, that is basically contains the observed reaction rate. So the observed reaction rate * the corresponding density, bulk density of the catalyst. So the bulk density of the catalyst is ρ_b is given by $1 - \phi \cdot \rho_c$, where ϕ is the

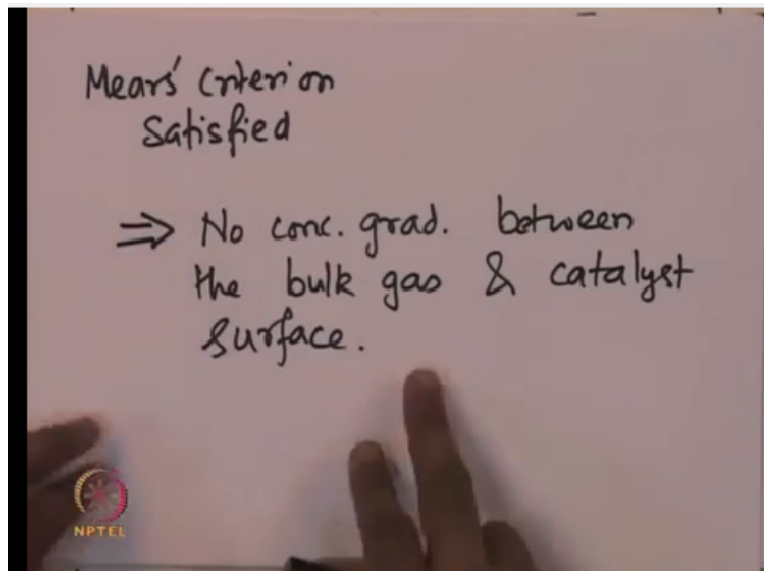
porosity of the batter is used and ρ_c is for a density of the catalyst.

So if we know what is the bulk density, then we can plug it in here and then we can find this expression and n is the order of reaction, n stands for the order of reaction, reaction order. And k_c is the corresponding mass transfer coefficient. k_c is the mass transfer coefficient. So one needs to estimate what is the mass transfer coefficient for transporting the species from bulk to the surface of the catalyst.

And then one needs to know what is the concentration of the species in bulk which is again a measurable quantity and one may also use different appropriate correlations. There are several correlations which are available to estimate the mass transport coefficient. One may use the appropriate correlation in order to estimate what is the value of this mass transport coefficient for the given conditions, that is for flow through packed beds.

So once we know these numbers, we will be able to estimate what is this quantity on the left hand side and if this is smaller than 0.15, then the external diffusion limitations are not playing any role and that can be ignored. If it is greater than 0.15, then certainly external diffusional limitations have to be taken into account.

(Refer Slide Time: 03:46)



So now if the Mears' criterion is satisfied, then this means that there is no concentration gradient

between the bulk gas and the external surface of the catalyst pellet. So there is no concentration gradient between the bulk gas and the catalyst surface if the Mears' criterion is satisfied. Now we looked at the concentration gradient, now one may ask what is the, what about the temperature gradient?

So can we get an estimate, can we find a criterion in order to know whether the temperature gradient, external temperature gradient, does it play a role, that is the gradient of temperature between the, temperature at the surface of the catalyst and the temperature of the bulk, does it play any role in limiting the reaction.

(Refer Slide Time: 04:53)

Mears' criterion 2

$$\left| \frac{-\Delta H_{Rx}(-r_A')\rho_b R E}{h T^2 R_g} \right| < 0.15$$

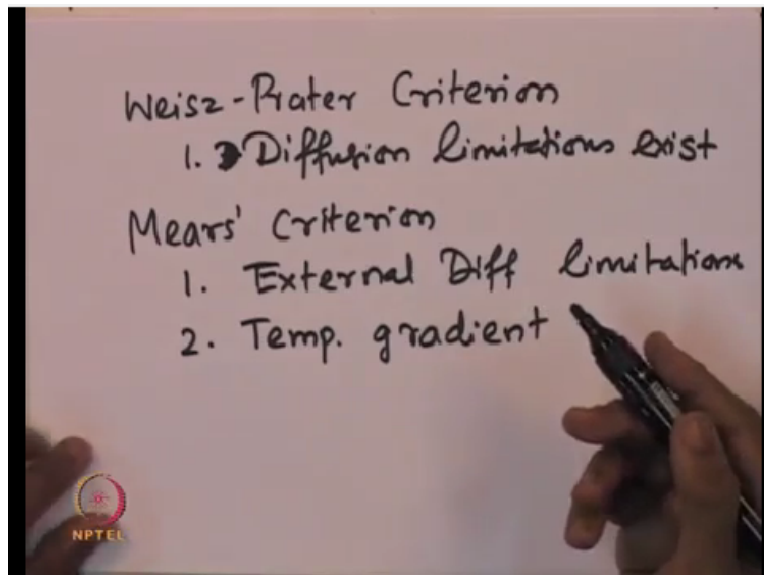
⇒ Bulk fluid temp
≈ Cat. surface temp.

So Mears' has come up with another criterion. So it is Mears' criterion 2. This suggests that if the modulus of this expression where ΔH is the heat of reaction $-r_A'$ which is the observed reaction rate ρ_b , which is the bulk density of the catalyst, R is the radius of the pellet that is used E corresponding heat transport coefficient.

There are several correlations which are available in order to estimate the heat transport coefficient, T^2 the square of the bulk temperature of the fluid stream and R_g the corresponding gas constant. So if this observed ratio, absolute value of this ratio, if that is less than 0.15, then it means that the temperature gradient does not play any role which means that the bulk fluid temperature is approximately equal to the catalyst surface temperature.

Note that intra-particle gradient need not necessarily be negligible; however, Weisz–Prater criterion can be used to identify when these gradients may be neglected. So this is an important criterion. So these 2 criterion can actually be used, these 2 criteria can actually be used in order to decipher whether the particular reaction is being conducted under diffusion limitations or not. So now let us summarize what we have learnt so far.

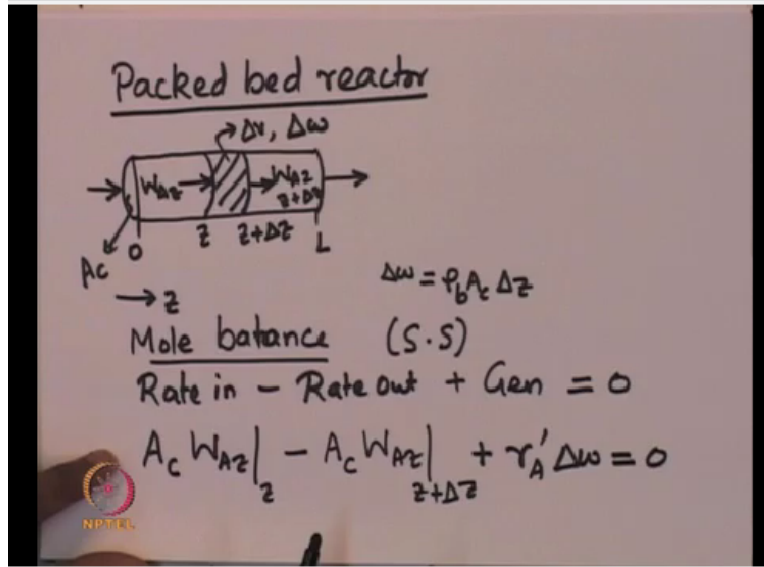
(Refer Slide Time: 06:28)



So we have looked at the Weisz–Prater criterion. And the first one is to decipher whether it is, Weisz–Prater criterion is basically to decipher if the diffusion limitations exist. And then we looked at the Mears' criterion. So the first criterion is basically to see if the external diffusional limitations exist, to check whether the external diffusional limitations exist and then the second one is to check whether the temperature gradient is important, external temperature gradient is important.

So these 3 criteria, Weisz–Prater criterion and the Mears' criterion, they play a very important role in real situations because if the experimental data is available, then this information can actually be used in order to decipher whether the reaction is being conducted under diffusion limitations or not. So next let us look at design of the packed bed reactor, as to how we can incorporate the concept of effectiveness factor in order in to the packed bed reactor design.

(Refer Slide Time: 08:00)



Now, let us consider a packed bed reactor. Packed bed reactor is essentially a tube filled with a catalyst and the fluid stream goes from one end of the tube into the other end of the tube. So let us consider a tube and there is a fluid stream which goes into this tube and it leaves the tube from this end. So if I mark this as $Z=0$, if Z is my coordinate system, so 0 to L , so L is the length of the reactor and if A_c is the cross-sectional area of the tube.

And now I can write a mole balance in order to capture the dynamics or the behaviour or the relationship of the conversion with all the other parameters. So now if I write a shell balance, I now identify a small shell which is filled with catalyst and let us assume that the volume of this shell is Δv and the amount of catalyst which is packed inside is Δw and if this, the location where this elements starts is Z and the location where it ends is $Z+\Delta Z$.

So this immediately means that Δw which is the differential amount of catalyst which is present in that location should be equal to the bulk density of the catalyst*the cross sectional area*the ΔZ which is the thickness of that particular element that we have chosen. So now we can write a mole balance for this small element.

And we can find out what is the model equation which captures the relationship between the concentration of the species which is undergoing the catalytic reaction with respect to other parameters. So suppose if the flux of species that enters this small element is $W_A Z$, that is the

flux that enters at that location.

And the flux that leaves is WAZ evaluated at $Z+\Delta Z$, so that is the flux that leaves that location. Then we can write a mole balance and the mole balance is essentially the molar rate at which the species enters that element-the molar rate at which the species leaves the element + whatever is generated, that will be equal to 0 under steady state conditions. So if you assume steady state conditions, then this is the balance that captures the process that is happening in this small element.

So what is the rate at which the species is getting into the element that is given by the cross sectional area A_c *the flux with which the species is actually entering into that element which is WAZ evaluated at that particular location, -the rate at which the species leaves is given by the cross sectional area*the flux at which the species leaves that element that is WAZ at $Z+\Delta Z$ and the generation is given by the reaction rate per unit rate of the catalyst*the amount of catalyst which is packed inside, that small element, ΔZ .

(Refer Slide Time: 11:50)

$$\Delta w = \rho_b A_c \Delta Z$$

$$A_c W_{AZ}|_Z - A_c W_{AZ}|_{Z+\Delta Z} + r'_A \rho_b A_c \Delta Z = 0$$

$$\frac{1}{A_c \Delta Z} [A_c W_{AZ}|_Z - A_c W_{AZ}|_{Z+\Delta Z} + r'_A \rho_b A_c \Delta Z] = 0$$

$$\text{Lt}_{\Delta Z \rightarrow 0} \Rightarrow \boxed{-\frac{dW_{AZ}}{dz} + r'_A \rho_b = 0}$$

So now we know that the, if the reactor volume is; we know that we can actually rewrite this expression as $\Delta w = \rho_b A_c \Delta Z$, that is the differential amount of catalyst that is packed inside that element and so we can now incorporate this into the model and therefore, the model will be $A_c WAZ - A_c AZ$ at $Z+\Delta Z$ + the rate*the bulk density*cross sectional area* $\Delta Z = 0$.

So that is the model. Now we can divide this whole equation by cross sectional area*delta Z. So that will be $1/Ac*\delta Z*Ac-Z+\delta Z+rA \text{ prime}*\rho b*Ac*\delta Z$, that is equal to 0.

So now if you take limit, delta Z going to 0, that if the element is very small, infinitesimally small, then the model equation becomes $-dWAZ/dZ+rA \text{ prime}*\rho b=0$. So this is the mole balance for species A which is undergoing a heterogeneous reaction in a packed bed reactor where WAZ is essentially the flux with which the species is actually entering the flux of the species at a particular location Z.

(Refer Slide Time: 13:43)

Handwritten notes on a whiteboard:

Total conc. of all species is constant
 C

$$W_{AZ} = \underbrace{-D_{AB} \frac{dC_{AB}}{dZ}}_{\text{Diffusion}} + \underbrace{y_{AB} (W_{AZ} + W_{BZ})}_{\text{Bulk flow}}$$

Superficial vel. U

$$W_{AZ} + W_{BZ} = C U$$

NPTEL logo is visible in the bottom left corner of the whiteboard image.

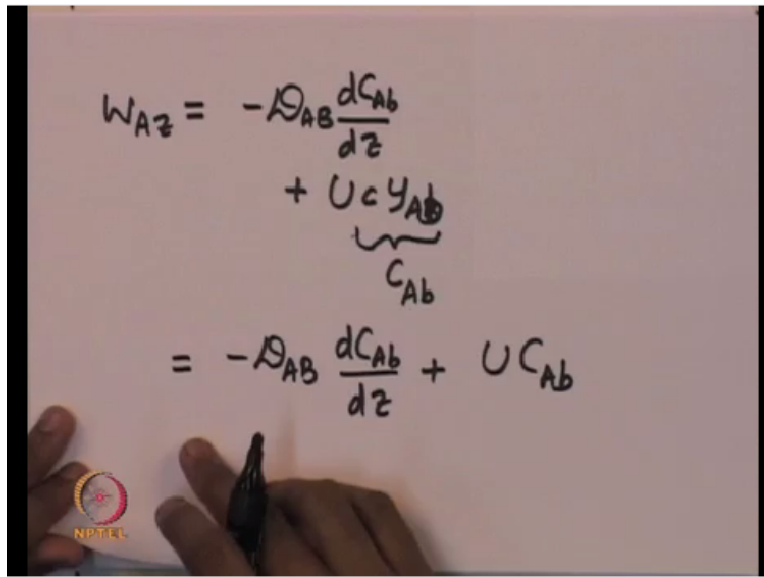
Now if I assume that the total concentration is constant, so if you assume that the total concentration of species, all species is constant, so total concentration of all species put together if it remains constant and if that value let us say is C. Now the flux with which the species crosses a particular location that can be written as $-D_{AB}$ which is the diffusivity of the species equimolar counter diffusivity of that species A * the concentration gradient dC_{AB}/dZ , $+y_{AB}$ which is the mole fraction of the species * the W_{AZ} which is the flux of the species at that location + the flux of species B at that location.

So now if we stare at this equation, the first term here corresponds to the diffusion term, correspond to the species diffusion and the second term corresponds to the bulk flow. Second term corresponds to the bulk flow which is like a convective transport and the first term

corresponds to the diffusive mode of transport.

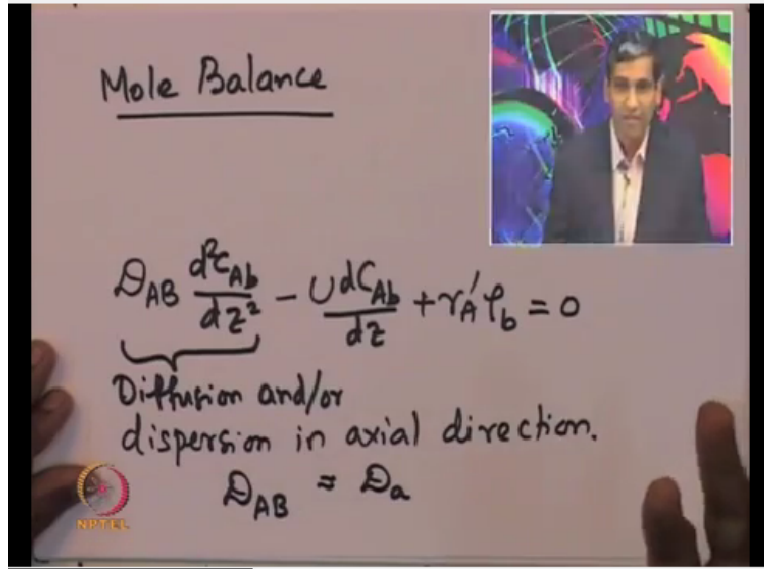
So now if we know what is the superficial velocity, so suppose if the superficial velocity is U , then the total flux that is crossing a particular location $W_{AZ} + W_{BZ}$, that should be equal to the total concentration C^* superficial velocity U . So now plugging in this expression, we can rewrite the expression for the flux of species that is W_{AZ} .

(Refer Slide Time: 15:56)


$$\begin{aligned}W_{AZ} &= -D_{AB} \frac{dC_{Ab}}{dz} \\ &\quad + U \underbrace{c_{y_{Ab}}}_{C_{Ab}} \\ &= -D_{AB} \frac{dC_{Ab}}{dz} + UC_{Ab}\end{aligned}$$

And that should be equal to $-D_{AB} \cdot dC_{AB}/dZ$, so that is the bulk concentration of the species at that particular location, $+U \cdot c^* y_{Ab}$, $y_{A \text{ bulk}}$, small b . So now if $c^* y_A$, $c^* y_A \text{ bulk}$ is nothing but the concentration of the species at that location. And therefore, it will be $-D_{AB} \cdot dC_{Ab}/dZ + UC_{Ab}$. So that is the expression for the flux of species that is crossing any particular location Z inside the reactor.

(Refer Slide Time: 16:42)



So now plugging in the expression for the flux in the mole balance, we can rewrite the mole balance as, so now the mole balance can be rewritten as D_{AB} which is the dispersion coefficient of the species, $\frac{d^2 C_{AB}}{dz^2}$. So that is the second differential of this concentration of the species, $-U$ which is the superficial velocity $\frac{dC_{AB}}{dz} + r_A'$ which is rate which the species is being consumed, rate at which the species is being generated ρ_b that should be equal to 0.

So now this first term here which is the diffusion into the second derivative of the bulk concentration of the species, so that is due to diffusion and; or it could be either because of diffusion, the transport of species is captured by this term, could be either because of pure diffusion or because of axial dispersion, because of dispersion in the axial direction.

So therefore for rest of the design equation, mole balances, we would consider D_{AB} which is the equimolar counter diffusivity, should be approximately equal to D_a which is basically the quantity that captures the extent of diffusion or the extent of dispersion or diffusion and dispersion together, okay. So here after we will refer to it is D_a in this lecture. So the modified mole balance using this representation is $D_a \frac{d^2 C_{AB}}{dz^2} - U \frac{dC_{AB}}{dz} + r_A' \rho_b = 0$.

(Refer Slide Time: 18:37)

$$D_a \frac{d^2 C_{Ab}}{dz^2} - U \frac{dC_{Ab}}{dz} + r'_A \rho_b = 0$$

$r'_A \Rightarrow f(C_{Ab})$

$\Omega \Rightarrow$ overall effectiveness factor

$$-r'_A = -r'_{Ab} \Omega$$

First order reaction

$$-r'_A = \Omega k'' S_a C_{Ab}$$

So now using this expression, now we need, in the next step, we need to do is we need to relate r_A to concentration. We need to find out what is this relationship with the concentration of the species.

(Refer Slide Time: 19:13)

$$\Omega = \frac{\eta}{1 + \eta k'' S_a \rho_b / k_c a_c}$$

$k_c \Rightarrow$ Mass transfer coefficient

$a_c \Rightarrow$ surface area / unit volume.

So suppose if ω is the overall effectiveness factor, if this is the overall effectiveness factor, so it is the overall effectiveness factor. Then the rate of reaction r_A prime can actually be given by $-r_A$ prime, can actually be, is given by $-r_A$ bulk, so this is the reaction rate in the catalyst. Now that should be equal to reaction rate if all the catalyst surface is now exposed and is present at the concentration of the species on the surface, then that will, concentration of species in bulk, then *overall effectiveness factor will actually be the actual reaction rate inside the catalyst.

So now if we assume that it is a first order reaction, if it is the first order reaction, then $-r_A$ prime is given by the effectiveness factor*the specific reaction constant*the surface area of the catalyst per gram, per unit weight of the catalyst, *the bulk concentration C_{Ab} .

(Refer Slide Time: 20:30)

$$D_a \frac{d^2 C_{Ab}}{dz^2} - U \frac{d C_{Ab}}{dz} - \Omega \rho_b k' S_a C_{Ab} = 0$$

C_{Ab} vs z

Flow through bed is large
 \Rightarrow axial dispersion: neglect

$$\left| \frac{-r_A' \rho_b d_p}{U_0 C_{Ab}} \right| \ll \left| \frac{U_0 d_p}{D_a} \right|$$

So now plugging in this expression into the mole balance, we can find that the mole balance is D_a which is the dispersion coefficient, $*d^2 C_{Ab}/dz^2 - U$, which is the superficial velocity, $*d C_{Ab} \text{ bulk}/dz - \Omega$ *the bulk density, $\rho_b * k'$ prime, which is the specific reaction constant, $*the surface area per gram catalyst * $C_{Ab} = 0$. So now if the flow through bed, so we need to solve this equation in order to find out the relationship between C_{Ab} and the how C_{Ab} , how the bulk concentration changes with location inside the reactor.$

So now suppose if the flow through the bed is large, suppose if the flow through the bed is significantly large, then one can actually neglect the axial dispersion. One can neglect the axial dispersion and that is not true always, only when the flow through bed is large and in fact, one can actually quantify what is the situation under which the axial dispersion can be neglected.

So the condition that has to be satisfied in order to assume that the axial dispersion can be neglected is given by $-r_A$ prime* ρ_b , which is the bulk density, $* the diameter of the particle/the superficial velocity. If that is much smaller than this quantity $U_0 d_p / D_a$, then it is$

acceptable to neglect the axial dispersion from the mole balance.

(Refer Slide Time: 22:29)


The image shows a whiteboard with handwritten mathematical equations. The first line shows the inequality $\Rightarrow \left| U \frac{dC_{Ab}}{dz} \right| \gg \left| D_a \frac{d^2 C_{Ab}}{dz^2} \right|$. The second line shows the differential equation $\Rightarrow \frac{dC_{Ab}}{dz} = - \frac{\Omega \rho_b k'' S_a}{U} C_{Ab}$. The third line shows the boundary condition $@ z=0, C_{Ab} = C_{Ab0}$. The final line shows the solution $C_{Ab} = C_{Ab0} \exp\left[-\frac{\Omega \rho_b k'' S_a}{U} z\right]$. In the bottom left corner of the whiteboard, there is a small circular logo with the text 'NPTEL' below it.

So this also suggests that the, so when axial dispersion can be neglected, it also suggests that $U \cdot dC_A/dZ$ which is the term that corresponds to the convective transport, that is significantly larger than the diffusive transport inside the packed reactor. So it suggests that the convective transport is larger than the diffusive transport and under these conditions, one can actually neglect the dispersion inside the reactor.

And so the modified mole balance which accounts for these assumptions is dC_A/dZ , that is equal to $-\omega$, and ω is the effectiveness factor $\cdot \rho_b \cdot k$, k is the reaction rate constant and S_a is the area of the catalyst per gram of the catalyst, surface area of the catalyst which is available/the superficial velocity $\cdot C_{Ab}$. So if suppose that at the entry of the reactor $Z=0$, if C_{Ab} =the sum constant value C_{A0} which is the concentration with which the species enters the reactor.

Then we can integrate this expression and find that $C_{Ab}=C_{Ab0} \cdot \text{exponential of } -\omega \rho_b S_a / \text{superficial velocity } U \cdot Z$. And/or we can use this expression in order to find out what is the conversion of the species in the reactor and the conversion is given by this expression here.

(Refer Slide Time: 24:16)

$$X = 1 - \frac{C_{Ab}}{C_{Ab0}}$$
$$X = 1 - \exp\left[-\frac{\Omega \rho_b k'' S_a Z}{U}\right]$$


Where $X=1-C_{Ab}/C_{Ab0}$ which is equal to $1-\text{exponential of } -\omega\cdot\rho_b\cdot k''\cdot S_a/U$, which is the superficial velocity, $\cdot Z$. So this expression captures the relationship between the conversion as a function of the location inside the reactor and so this is very useful in terms of estimating what is the reaction, what is the conversion given the overall effectiveness factor and the system parameters and the configuration of the reactor that is what is the particle diameter, etc.

So what we have seen in today's lecture is we have looked at the criterion for when the internal diffusion is important and when the external diffusional limitations are important and that is simply based on the experimental data that has been obtained from the real reactor system and also we have attempted to see how to incorporate the effectiveness factor into the mole balance of the packed bed reactor in order to find out what is the, how the conversion changes as a function of position in the packed bed reactor. Thank you.