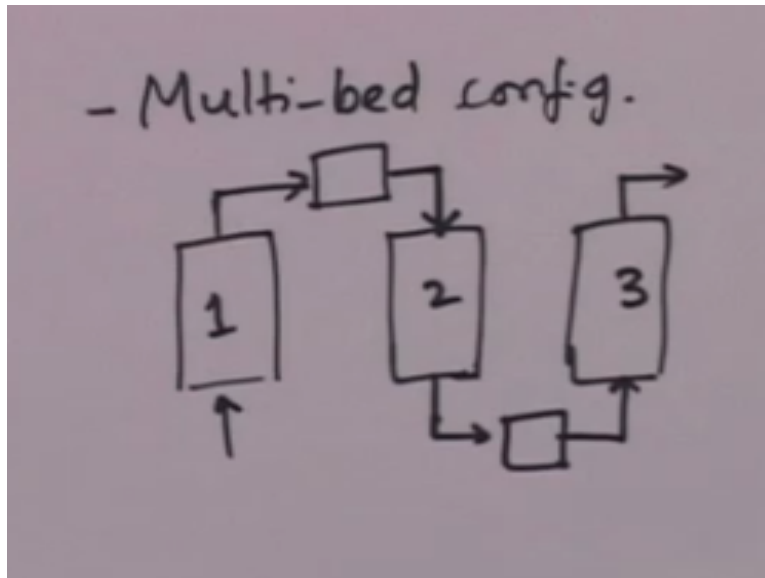


Chemical Reaction Engineering - II
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Lecture – 38

Packed-Bed Reactor Design: External and Internal Resistances

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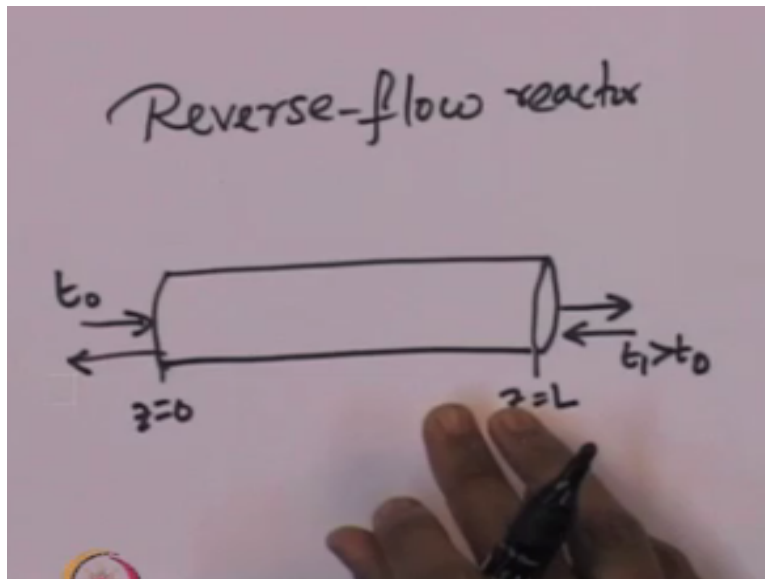
Now, the packed bed reactor also is being operated under a different configuration, there are several configurations that have been used in the industry and some of these are multi bed reactor, so multi bed configuration. In a multi bed configuration, there are multiple beds which are present, there are multiple tubular reactors, where the fluid stream goes into one reactor and then there may be some unit operation that may be present in between.

Let us say to separate something or it may be to heat the fluid or any other unit operation and whichever is required and from there, the input goes into the second reactor and then from the second reactor, the fluid stream leaves and then there may be some other unit operation if it is required otherwise, it goes directly into the third stream so on and so forth, so it is a multi-bed reactor where the fluid stream constantly goes from reactor 1 to reactor 2, reactor 3 etc.

And while going through this, the conversion increases and hopefully at the end of the multi bed the desired conversion is achieved and this is done for various reasons for example, the nature of the catalyst might be required might be different, if the temperature conditions at

which the reaction is conducted is different so therefore, one may actually pack a different catalyst in each of these multiple bed and so that way a desired conversion can be achieved.

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And as well the catalyst deactivation can be prevented so, another very well-known configuration is called the reverse flow reactor configuration, so reverse flow reactor configuration, so in the reverse flow reactor configuration what is done is; suppose if this is a tubular packed bed reactor now, the fluid is flowing let us say this is at $z = 0$, so this is the entry point at certain time and this is $z = l$.

So at a certain time t , the fluid enters the reactor at $z = 0$ and then it leaves the reactor in $z = l$, at a later time t_1 , let us say if this is t_0 at a later time t_1 which is $> t_0$, the fluid is now entering from into the reactor from the; from $z = l$ and it flows in the reverse direction and then leaves the reactor at $z = 0$, so this is at time $t = t_1$, so this kind of a switching of the direction of flow is done at a certain frequency.

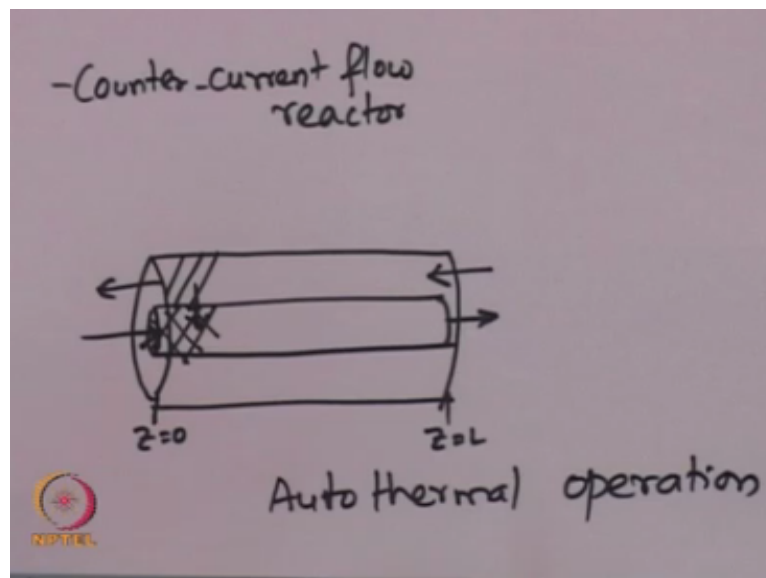
And this is very useful if the catalyst deactivation has to be prevented for example, when an exothermic reaction is conducted inside the packed bed reactor, there is a constant increase in the temperature because of the inside the reactor because of the heat that is being liberated by the reaction while it is happening and due to which the temperature at the other end of the reactor that is the downstream of the reactor, the temperature is likely to increase significantly.

Now, in order to and that may actually deactivate the catalyst or it may leave post some severe safety problems in order to prevent that at a certain pre-set frequencies if the fluid stream is

now the direction of the fluid stream is reverted then the temperature front which is actually generated because of the exothermicity of the reaction is now preserved inside the reactor itself and which may also be used to preheat.

And as a by-product there are, most part of the reactor will not be exposed to a certain very high temperatures and this can actually prevent the deactivation of the catalyst and this provides a very useful mechanism to protect the catalyst which is very expensive, so this is a very well well-known configuration and the other configuration which is also fairly used particularly, if you want if the reactant feed stream is of a lean concentration if the concentration of the reactant is very small in the feed then, counter current flow reactor is being used.

(Refer Slide Time: 04:47)



So, a counter current flow reactor is essentially a 2 chamber reactor, so it will be 2 concentric cylinders, now in this concentric cylinder, the feed stream is flown in one direction in one chamber and in the other direction in the other chamber so, the fluid stream is now flown at a in a counter current fashion where the fluid stream in the inside tube leaves first, enters the reactor at $z = 0$ and leaves the reactor at $z = 1$.

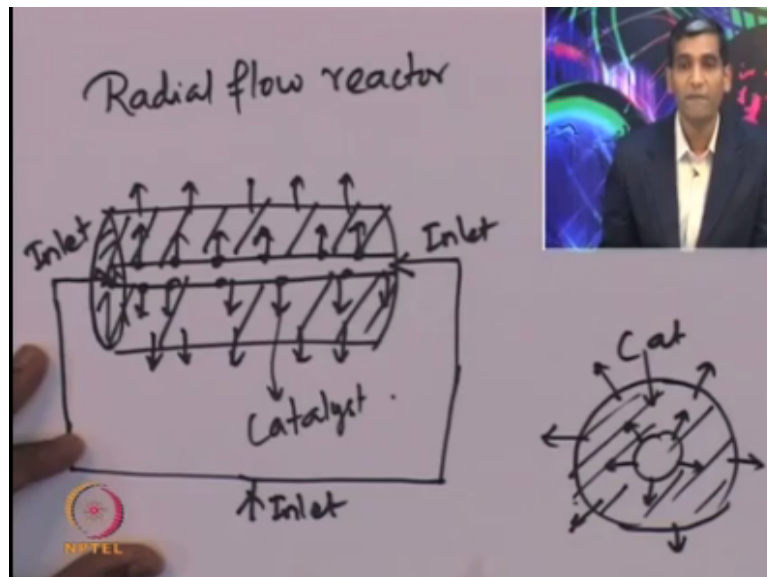
While the fluid stream in the outside concentric cylinder, external cylinder enters at $z = 1$ and leaves at $z = 0$, so this has a unique advantage that if the concentration is very lean then it can be this kind of a configuration can actually be used to preheat the fluid which increases the reaction rate remember that the reaction rate is increases, if it is an exothermic reaction then the reaction rate actually increases as a function of temperature.

And therefore, if the; if we have a counter current flow then, the feed stream which is present near the inlet of the reactor in the inside tube can actually obtain heat from the fluid stream which leaves the reactor from the outside chamber and because the conversion of the fluid stream near the exit is expected to be high and as a result the fluid stream also is expected to carry a lot of heat while it leaves the reactor.

So, in order not to lose the heat that it is gained because of the reaction such a counter current flow reactor provides a mechanism by which the heat can be transferred from the outside chamber to the inside chamber and the inside chamber to the outside chamber wherever it is desirable so, such kind of an operation where simultaneous heat transport from 2 chambers into each other and an exothermic reaction is what is called as Auto thermal operation of a packed bed reactor.

So, such kind of a reactor is very useful if the reactant concentration is very lean and yet the desired conversion is required, yet another configuration which is also being used in industry is called the radial flow reactor.

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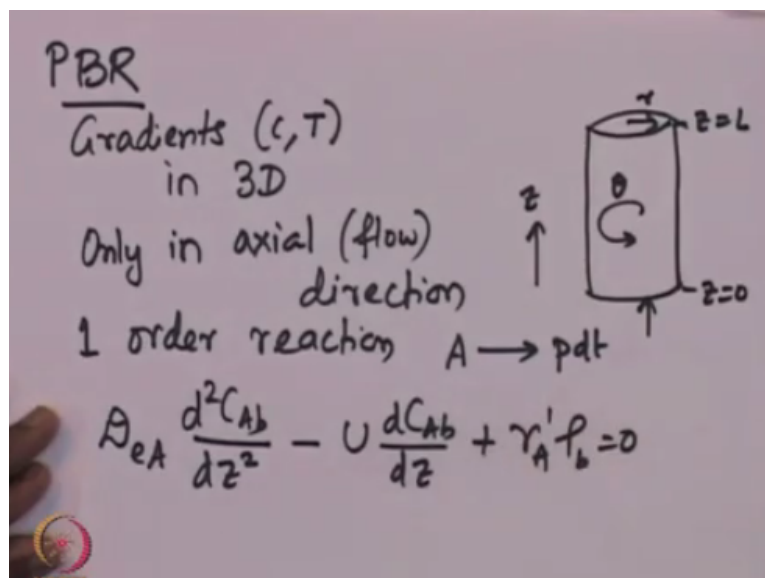
So, in a radial flow reactor what happens is; suppose if this is the tube and there is a small concentric channel which is present inside the reactor and the space between the concentric channel inside and the exterior of this tube is actually filled with catalyst now, the fluid stream which is fluid stream containing the reactant is made to flow through the inside chamber from both sides, the fluid stream flows simultaneously from both sides, inlet fluid stream.

Now, when it flows from both sides, a sparger is kept along the periphery of the inside tube, these are tiny holes which are placed at a certain pre calculated distance and so the fluid stream which enters through the reactor on either side they leave, they go into the chamber which contains the catalyst particle through this sparger, so the feed stream is sparge uniformly in all directions inside the radial flow reactor.

And the reaction happens in the catalyst and then the fluid stream leaves from the curved surface of this exterior tube, so this is what is called as a radial flow reactor at a side view of this reactor it looks like this, so if I take a cross section of this reactor and make a side view of it then, I can see that the fluid stream actually leaves from the inside tube uniformly in all directions.

And then the catalyst is present here, so that is the catalyst and the reaction happens in the region where the catalyst is packed and the fluid stream leaves from the exterior of this chamber so, this kind of an operation is what is called as a radial flow reactor configuration and that also is being used in many different types of situations. The main advantage of this configuration is that it facilitates operation under low pressure drop.

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So, let us look at the design of packed bed reactor; let us look at a packed bed reactor design now the, in a tubular reactor a packed bed reactor is essentially a tube in which the catalysts are packed so therefore, the temperature in the concentration gradient is expected to be present in the axial direction if this is the flow of the fluid then it is expected to be present in the direction of the flow of the fluid which is called the axial direction.

And then it is also expected, the gradients are expected to be present in both the radial direction and the angular direction so, in principle the temperature and the concentration gradients are expected to be present in all 3 dimensions and it is only concentration gradients if the reactor is operated under isothermal conditions. So, therefore the gradients concentration and temperature in all 3 dimensions, it is present in all 3 directions.

However, for the purpose of design we will assume that the gradients are present only in the axial direction; axial that is essentially flow direction, we will assume that the gradients are present only in the flow direction. So, now for this situation we have already written the mole balance in one of the lectures before so, if the reaction is a first order reaction then the mole balance essentially is axial dispersion coefficient DeA .

If A is the reaction which is leading to product formation, then DeA the axial dispersion coefficient multiplied by $d^2 C_{AB}$ which is the concentration of the species in bulk divided by dz^2 that is the that captures the diffusion of species in the reactor in the axial direction - $u * dC_{AB}/ dz + r_A \text{ prime} * \rho_b = 0$. Now for; so let us draw the coordinates, so if suppose if this is the tubular reactor, suppose this is the tubular reactor then this is the z direction and this is the radial direction.

And then the angular direction is let us call it θ , so θ is the angular direction, so there are no gradients we assume that there are no gradients in the θ and the r direction and the gradients are present only in the z direction, so this correspond the; first term here corresponds to the diffusion in the z direction and the flow is happening from $z = 0$ to $z = l$, so the gradients are the; the first term here corresponds to the diffusion in the direction of flow.

And the second term corresponds to the bulk convection in the direction of the flow and third term corresponds to the rate at which the species A is being consumed to form the necessary product.

(Refer Slide Time: 13:13)

$$-r_A' = \Omega K'' S_a C_{Ab}$$

$$\Omega = \frac{\eta}{1 + \eta K'' S_a \rho_b / K_c a_c}$$

Flow is large

$$\left| D_{eA} \frac{d^2 C_{Ab}}{dz^2} \right| \ll \left| u \frac{dC_{Ab}}{dz} \right|$$

So suppose, if we know the overall effectiveness factor then, we can write the reaction rate as $-r_A'$; $-r_A'$ prime equal to the overall effectiveness factor multiplied by the corresponding specific reaction constant into the surface area per unit weight of the catalyst multiplied by the bulk concentration C_{Ab} .

Now, for a first order reaction, the overall effectiveness factor is given by the local effectiveness factor η divided by $1 + \eta * K''$ multiplied by the surface area of the catalyst per gram of catalyst multiplied by the bulk density of the catalyst divided by the mass transport coefficient into area per unit volume of the catalyst.

So that gives the reaction rate in terms of the measurable quantity such as the bulk concentration of the species which is reacting to form the necessary products and so now, we can suppose, if we assume that the flow through the bed is significant if the flow is large then, we can assume that the diffusion has done before we can assume that the diffusion of species in the bed is significantly smaller compared to the bulk flow of the fluid.

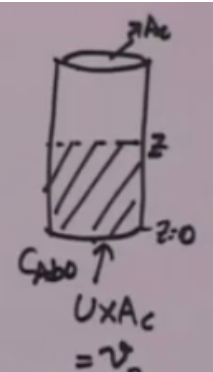
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$$\frac{dC_{Ab}}{dz} = - \left(\frac{\Omega \rho_b K'' S_a C_{Ab}}{u} \right)$$

$$\omega = \rho_b A_c z$$

$$\frac{dC_{Ab}}{d\omega} = \frac{-\Omega \rho_b K'' S_a C_{Ab}}{u \rho_b A_c}$$

$$= \frac{-\Omega K'' S_a C_{Ab}}{v}$$

$$v = v_0; @ \omega = 0, C_{Ab} = C_{Ab0}$$


So, under this condition we can actually, we can rewrite the mole balance as dC_A/dz ; dC_A bulk/ dz that is = - ω * ρ_b , which is the bulk density of the catalyst * K double prime * S_a * C_{Ab} divided by u . Now, sometimes the design parameter that one needs to estimate may be the weight of the catalyst or in sometimes it may be the size of the reactor given a certain conversion.

So, therefore we can actually convert this equation in terms of the weight of the catalyst, so the weight of the catalyst that is packed in a certain location in the actual direction is given by the bulk density of the catalyst multiplied by the cross sectional area of the reactor multiplied by the corresponding position. So, if this is the tubular reactor and let us say, we are looking at this particular z and if the cross sectional area is A_c , cross section area of the reactor is A_c .

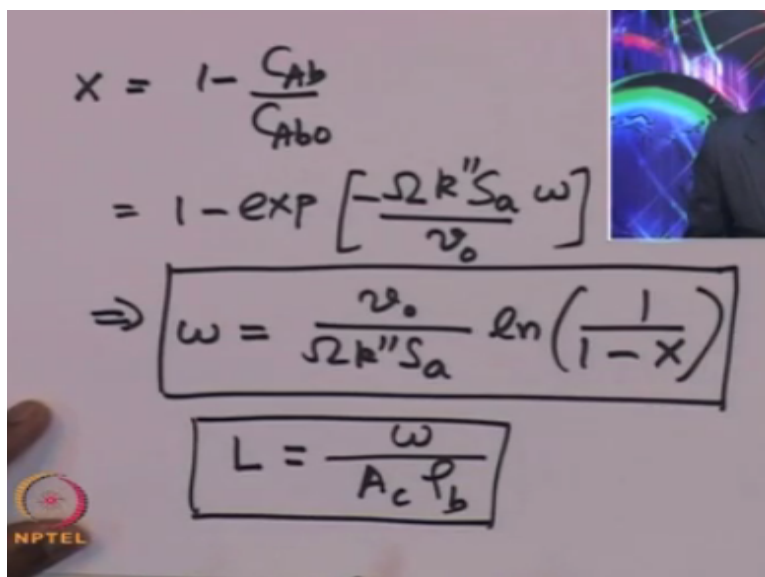
Then we want to know what is the total amount of weight of catalyst that is packed from $z = 0$ to up to a some particular point z , so that is given by ρ_b which is the bulk density of the catalyst multiplied by the cross sectional area into z which gives the volume of the reactor till that location and therefore, we can rewrite the model equation as dC_{Ab}/dW that is = - overall effectiveness factor * ρ_b * K double prime $S_a C_{Ab}$ divided by u * ρ_b * A_c .

So that is because of the dependence of this weight of the catalyst on the density and the cross sectional area and that is why we get these 2 terms here, so we can cancel out these 2 and u * A_c , if u is the superficial velocity with which the fluid is entering the reactor u * A_c which is the cross sectional area will give you the volumetric flow rate with which the fluid stream is entering the reactor.

So, therefore this can be written as - overall effectiveness factor * S_a divided by the volumetric flow rate C_{Ab} , so the volumetric flow rate at the inlet could be v_0 and the volumetric flow rate at that particular location if there is volume expansion then, the volumetric flow rate at that particular location could be different. So, if you assume that there is no volumetric expansion then we can assume that $v = v_0$.

And if and also if we assume that at; and if you assume that at if the weight of the catalyst is 0, then the C_{Ab} which is the bulk concentration that is equal to the concentration with which the fluid actually is entering the reactor, so C_{Ab0} is the concentration with which the fluid is actually entering the packed bed reactor in which the reaction is happening.

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The image shows a whiteboard with handwritten mathematical equations. The equations are:

$$X = 1 - \frac{C_{Ab}}{C_{Ab0}}$$

$$= 1 - \exp\left[-\frac{\Omega K'' S_a w}{v_0}\right]$$

$$\Rightarrow \boxed{w = \frac{v_0}{\Omega K'' S_a} \ln\left(\frac{1}{1-X}\right)}$$

$$\boxed{L = \frac{w}{A_c \rho_b}}$$

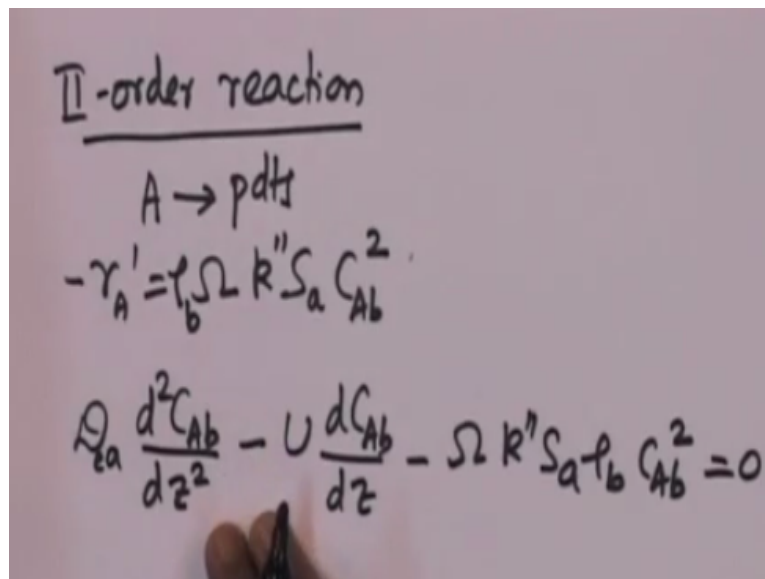
In the bottom left corner of the whiteboard, there is a small logo for NPTEL (National Programme on Technology Enhanced Learning).

This equation can now be integrated to find that the conversion X is given by $1 - C_{Ab}/ C_{Ab0}$ and that is $= 1 - \text{exponential of } - \text{omega which is the overall effectiveness factor multiplied by } K \text{ double prime multiplied by the surface area of the catalyst available for the reaction per unit gram of catalyst multiplied by } w \text{ divided by the volumetric flow rate } v_0 \text{ with which the fluid is actually entering the reactor.}$

Or we can rewrite this as $w = v_0$ divided by $\text{omega } K \text{ double prime } S_a * \log \text{ of } 1/ 1 - X$, so this provides the relationship between the weight of the catalyst that is required for a specified conversion, if we specify the conversion then we can find out how much weight of catalyst is required. So, if we know the weight of the catalyst then we should be able to find out what should be the length of the reactor which is required for a given cross section.

And that can be found simply by using this relationship, the length of the reactor is given by weight of the catalyst divided by the cross sectional area * density, so this method provides a mechanism, this design provide the mechanism by which for a specified conversion, if the assumption that the bulk flow is significantly larger than that of the diffusion then, we can actually find out what is the weight of the catalyst which is required for a given conversion and what is the length of the reactor for a specified conversion.

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So suppose, if we look at a second order reaction suppose, if we consider a second order reaction; a second order reaction and if A going to products is the reaction scheme and if $-r_A'$ prime is the rate at which the species A is being consumed if that is given by the overall effectiveness factor ω multiplied by the corresponding specific rate constant K double prime into the surface area of the catalyst per unit weight of the catalyst * C_{Ab} square, so that is the rate law.

And the mole balance for the reactor will be D_a which is the dispersion coefficient of the species * $d^2 C_{Ab} / dz^2$ that is the diffusion term which with the rate at which the species is diffusing inside the reactor and $-u$ times $d C_{Ab} / dz$ - $\omega * K$ prime * $S_a * \rho_b * C_{Ab}$ square, so it should be a ρ_b here, so the that is the mole balance which captures the dependence or the that captures the dependence of the concentration of the bulk concentration of the species as a function of position and other parameters of the system including the specific rate constant.

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$$\begin{aligned}
 & \left| D_{eff} \frac{d^2 C_A}{dz^2} \right| \ll \left| u \frac{dC_{Ab}}{dz} \right| \\
 \Rightarrow & \frac{dC_{Ab}}{dz} = - \frac{\Omega K'' S_a \rho_b C_{Ab}^2}{u} \\
 \Rightarrow & \rho_b A_c \frac{dC_{Ab}}{dw} = \frac{-\Omega K'' S_a \rho_b C_{Ab}^2}{u A_c \rho_b} \\
 \Rightarrow & \frac{dC_{Ab}}{dw} = - \frac{\Omega K'' S_a C_{Ab0} (1-X)^2}{v} \\
 & C_{Ab} = C_{Ab0} (1-X)
 \end{aligned}$$

So, now we can solve this if we assume once again that the bulk flow is significantly larger than the corresponding diffusion rate then, the DA square is significantly smaller to the corresponding bulk flow then, the mole balance will simply be reduced to $dC_A \text{ bulk} / dz$ that is = - overall effectiveness factor Ω multiplied by K double prime * S_a * ρ_b * C_{Ab} square divided by u .

Now, once again we can reformulate this in terms of the dependence of the concentration of bulk species concentration of species A in bulk as a function of the weight of the catalyst, so we can rewrite this as $\rho_b A_c * dC_{Ab} / dw$ which is the; where small w stands for the weight of the catalyst and that is = - ΩC_{Ab} square divided by $u * A_c * \rho_b$ that is the bulk density of the catalyst.

And so from here, we can find that dC_{Ab} / dw that should be = - ΩK double prime S_a divided by the volumetric flow rate v multiplied by $C_{Ab0} * 1 - X$ the whole square, so this expression provides a relationship between the concentration of the species and other parameters and where $C_{Ab} = C_{Ab0} * 1 - X$ where X is the corresponding conversion.

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$$v = v_0 ; \text{ @ } z=0 \Rightarrow w=0$$

So, now we can also incorporate the relationship between the concentration and conversion on the left hand side of the expression and we can integrate the equation as by assuming that the volumetric flow rate at any location is equal to the inlet volumetric flow rate by assuming that the volume changes are negligible and also by assuming that at $z = 0$, the weight of the catalyst is 0 that is there are no catalysts before the reactor starts.

And the reaction is actually happening inside the reactor, this differential equation cannot be integrated analytically as in the case of a first order reaction, this is because the overall effectiveness factor for this case will be a function of conversion. So, now such kind of a design can actually be used for various kinds of reactions, it could be; such kind of a design can be performed for rate law which is non-monotonic that is it is a non nth order type reaction.

One could actually write a design equation for adsorption inhibition type reactions, for (()) (23:55) type reactions and such kind of a reaction can; design equation can also be written for situations where multiple species are actually participating in the reaction, so it is a good time to summarize that what we have seen so far is we have looked at various criterion for deciphering what is the what; how deciphering from experiments; experimental conditions whether the reaction is actually internal diffusion limited or external diffusion limited or surface reaction limited.

Also, we have looked at what is the recipe; general recipe for performing the reactor design and also performed the, looked at the reactor design equations for a first order and a second order reaction, thank you.