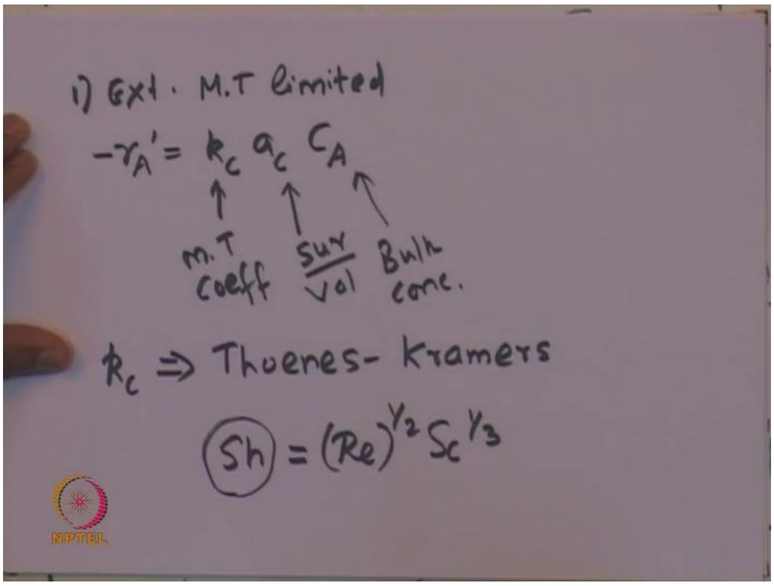
Chemical Reaction Engineering II
Prof. Ganesh Vishwanathan.
Department of Chemical Engineering
Indian Institute of Technology, Bombay

Lecture -17
Packed-bed reactor design

Friends, let us look at how to obtain the limiting cases from the experimenter data. That is what whether the reaction is under diffusional limitations or under the surface reaction limiting conditions and how it depends upon various parameters of the system.

(Refer Slide Time: 00:50)



1) Ext. M.T limited

$-r_A' = k_c \; a_c \; C_A$

m.T coeff

sur/vol

Bulk conc.

$k_c \Rightarrow$ Thoenes- Kramers

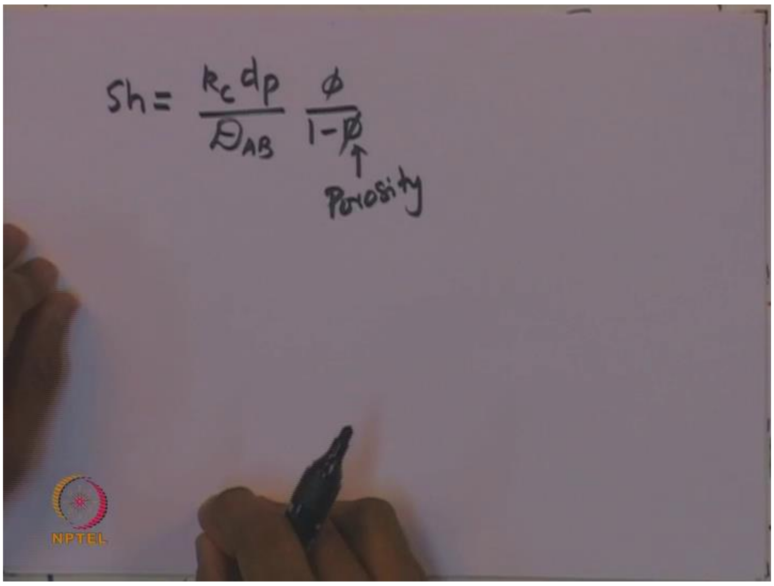
$\boxed{Sh} = (Re)^{1/2} Sc^{1/3}$

So, first let us consider the external mass transport limited case. Now, where in the extra under the external mass transport limitations the reaction rate is given by kc ac into CA where, kc is the mass transport coefficient; ac is the surface to volume ratio and CA is the bulk concentration. Now, kc can be estimated using appropriate correlation such as the Thoenes Kramer correlation can be estimated using Thoenes Kramer’s correlation.

Now, the correlation is as follows it says that the Sherwood number should be equal to Reynolds number to the power of half multiplied by the Schmidt number to the power of 1 by 3. So, the mass transport coefficient is embedded in Sherwood number, while other properties like velocity etcetera they are all embedded in Reynolds number and the Schmidt number.

So, now looking at the functional form of these 3 terms, we would be able to discern how the mass transport coefficient depends upon various parameters such as the diameter of the particle or the temperate of the temperate at which the reaction is being conducted etcetera. And, then find out what is the relationship or functional dependence of the overall reaction rate on various systems parameters such as, the diameter of the particle and velocity of the velocity with which the fluid is flowing into the rector.

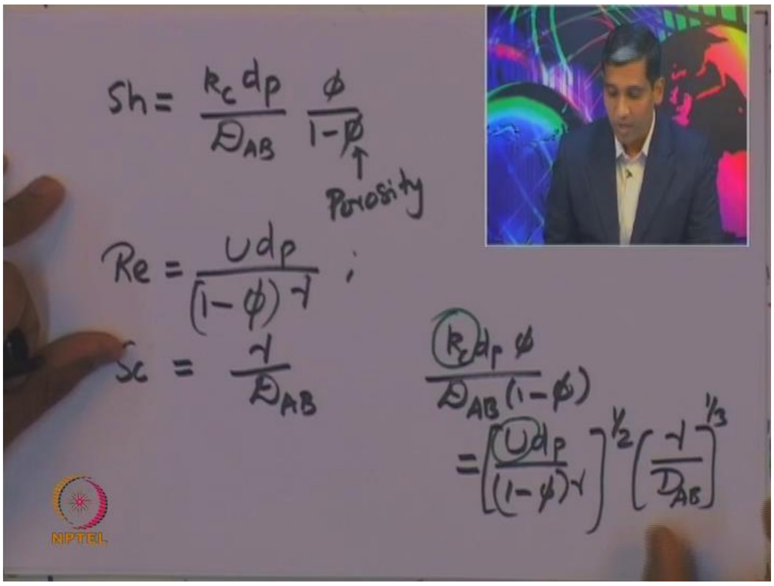
(Refer Slide Time: 02:37)



$$Sh = \frac{k_c d_p}{\mathcal{D}_{AB}} \frac{\phi}{1-\phi}$$

So, now if I look at the expression for Sherwood number, you see that the Sherwood number is given by mass transport coefficient kc multiplied by the diameter of particle dP divided by the equimolar counter diffusivity with DAB multiplied by phi divided by 1 minus phi. Here, phi is refers to porosity of the bed and it does not represent the Thiele modulus. Here, 5 is the porosity of the bed.

(Refer Slide Time: 03:03)



$$Sh = \frac{k_c d_p}{D_{AB}} \frac{\phi}{1-\phi}$$

Porosity

$$Re = \frac{U d_p}{(1-\phi)\nu} ;$$

$$Sc = \frac{\nu}{D_{AB}}$$

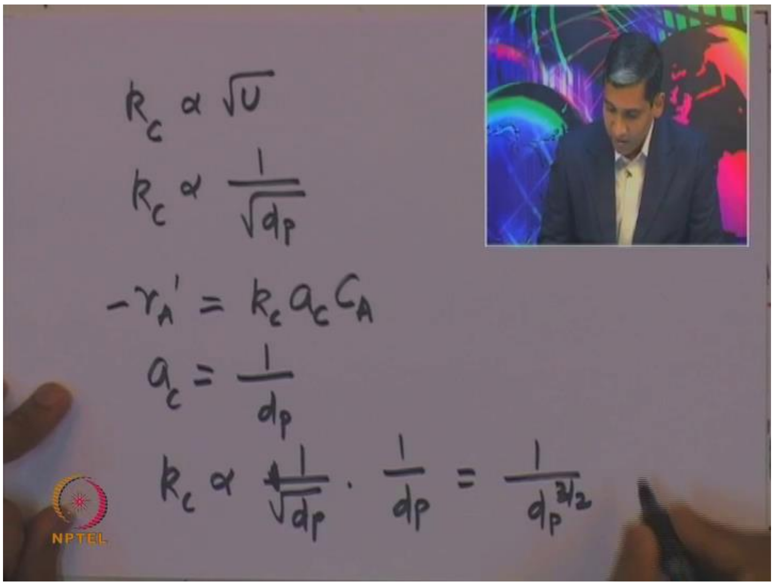
$$\frac{\boxed{k_c} d_p \phi}{D_{AB}(1-\phi)} = \left[\frac{\boxed{U} d_p}{(1-\phi)\nu}\right]^{1/2}\left[\frac{\nu}{D_{AB}}\right]^{1/3}$$

Reynolds number is given by U times dP. U is the superficial velocity, dP is the diameter of the particle diameter of the catalyst palette in which the catalytic reactions being conducted. Divided by the 1 minus phi where phi is porosity into nu which is kinematic viscosity. And similarly, Schmidt number is given by kinematic viscosity divided by the equimolar counter diffusivity of the species a that is of interest.

So, from here we can now write the all these plug in all this expression in the Thoenes Kramer correlation. We find that kc dP into phi divided by DAB into 1 minus phi. That should be equal to U dP by 1 minus phi into nu to the power of half multiplied by nu by DAB to the power of 1 third. So, that is the a dependence of the mass transport coefficient where, here kc is the first be the mass transport coefficient. And this is the functional dependence of mass transport coefficient on the terminal velocity U and Dp and other parameters.

So, from here we can discern that the mass transport coefficient k is now of a proportional to just kc is proportional to square root of U, where U is it a superficial velocity and also it is proportional to 1 by square root of dP kc is proportional to 1 by square root of dP.

(Refer Slide Time: 05:12)



$$k_c \propto \sqrt{U}$$

$$k_c \propto \frac{1}{\sqrt{d_p}}$$

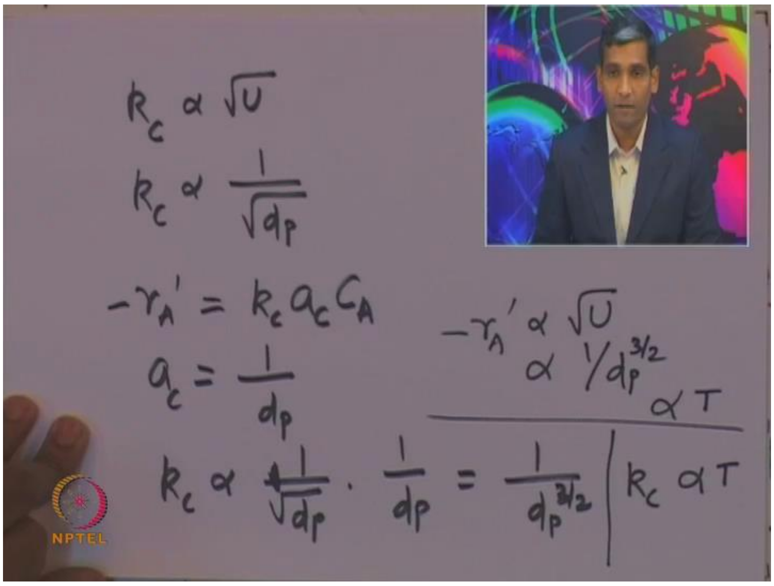
$$-r_A' = k_c a_c C_A$$

$$a_c = \frac{1}{d_p}$$

$$k_c \propto \frac{1}{\sqrt{d_p}} \cdot \frac{1}{d_p} = \frac{1}{d_p^{3/2}}$$

Now, if a look at the reaction rate, reaction rate this kc into surface area per unit volume multiplied by the corresponding concentration CA. So, now, the from here we can see that the area per unit volume is given by 1 by Dp. And therefore, the reaction rate therefore, the mass transport coefficient kc is proportional to square root 1 by square root of dP into 1 by dP. So, that could be given by 1 by dP to the power of 3 by 2. So, that is the functional form of the mass transport coefficient on the diameter of the particle. So, it is dP the power of 3 by 2. Now, similarly 1 can see that the mass transport coefficient is typically proportional to the temperature at which the reaction is being conducted.

(Refer Slide Time: 05:40)



$$k_c \propto \sqrt{U}$$

$$k_c \propto \frac{1}{\sqrt{d_p}}$$

$$-r_A' = k_c a_c C_A$$

$$a_c = \frac{1}{d_p}$$

$$k_c \propto \frac{1}{\sqrt{d_p}} \cdot \frac{1}{d_p} = \frac{1}{d_p^{3/2}}$$

$$k_c \propto T$$

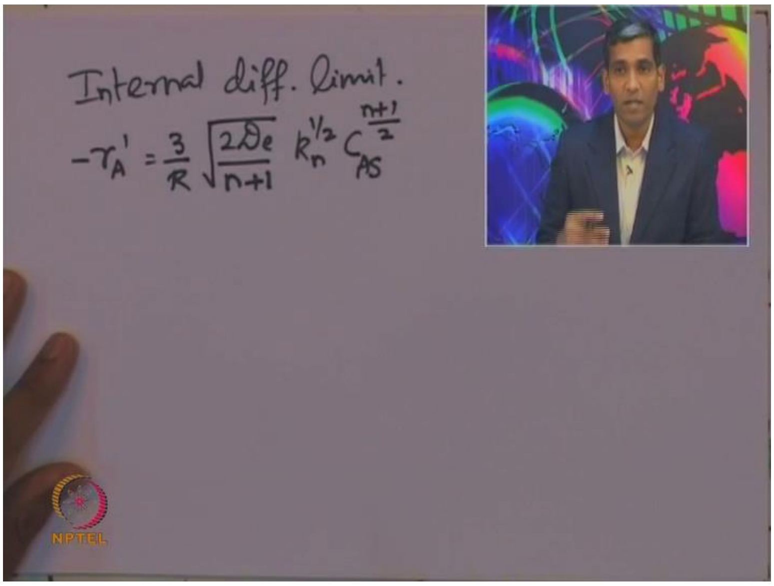
$$-r_A' \propto \sqrt{U}$$

$$\propto 1/d_p^{3/2}$$

$$\propto T$$

So, therefore, from here we can see in that the reaction rate. Reaction rate is proportional to square root of U, which is the superficial velocity with which the fluid is flowing into the reactor and also its proportional to 1 by dP to the power of 3 by 2 and it is also proportionate to the temperature at which the reaction reactor is being operated. So, that provides the functional form of the reaction rate; a dependence of the reaction rate on various parameters of the system.

(Refer Slide Time: 06:23)

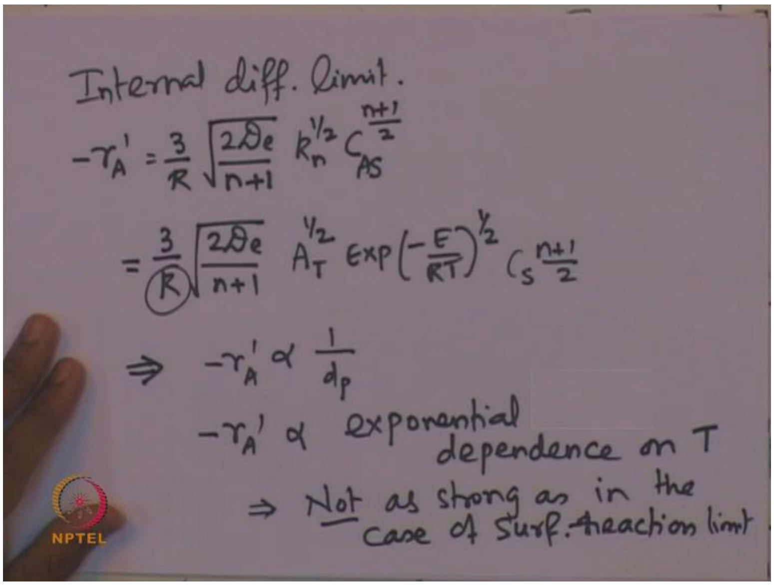


Internal diff. limit.

$$-r_A' = \frac{3}{R}\sqrt{\frac{2\mathcal{D}_e}{n+1}}\, k_n^{1/2}\, C_{AS}^{\frac{n+1}{2}}$$

So, therefore, now next if we look at the internal diffusional limitation; if you look at the internal diffusional limitations, then the reaction rate is for any n-th order reaction is given by r a prime is equal to 3 by r that is the radius of the pellet catalyst pellet that is being used into square root of 2 times the diffusivity, effective diffusivity of the species divided by n plus 1 multiplied by kn to the power of half. Where, k is the n-th order reaction rate constant multiplied by the surface concentration CAS to the power of n plus 1 by 2. So, that is the rate law.

(Refer Slide Time: 07:19)



Internal diff. limit.

$$-r_A' = \frac{3}{R}\sqrt{\frac{2D_e}{n+1}}\, k_n^{1/2}\, C_{AS}^{\frac{n+1}{2}}$$

$$= \frac{3}{\textcircled{R}}\sqrt{\frac{2D_e}{n+1}}\, A_T^{1/2} \exp\left(-\frac{E}{RT}\right)^{1/2} C_S^{\frac{n+1}{2}}$$

$\Rightarrow -r_A' \propto \frac{1}{d_p}$

$-r_A' \propto$ exponential dependence on T

⇒ Not as strong as in the case of surf. reaction limit

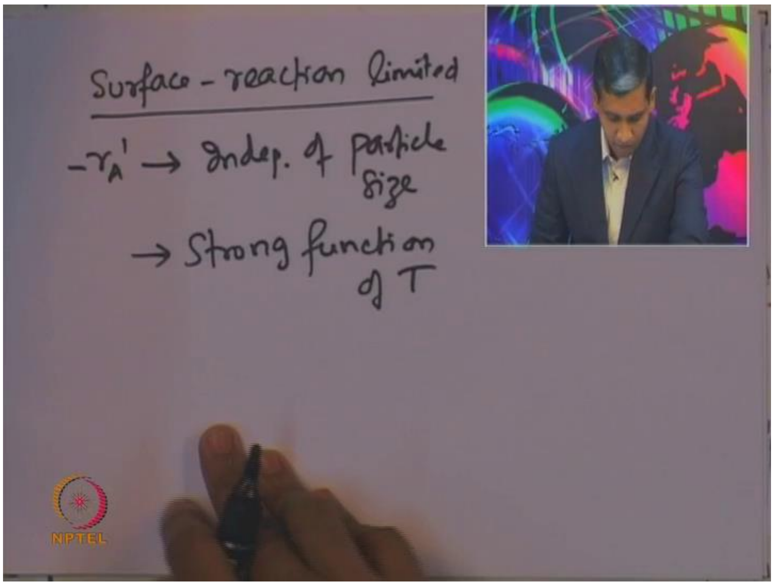
Now, the rate constant actually follows Arrhenius type dependence on the temperature. So, therefore, we can rewrite this expression as 3 by r into square root of 2 times De divided by n plus 1 multiplied by the frequency factor AT to the power of half into exponential of minus E by RT to the power of half in go CS to the power of n plus 1 by 2. So, that is the expression. So, given that the where E is the activation energy and T is the temperature at which the reactor is being operated.

So, from here 1 can discern that the rate of reaction rA is proportional to 1 by diameter of the particle dP, because of this functional dependence on because of this term 3 by r. And also the rate of reaction is has an exponential dependence on the temperature, on the temperature at which the reactor is being operated. It is important to also note that diffusivity is also a function of temperature.

So, this suggests that the unlike in the case of external mass transport control situation the entire diffusion controlled situation the reaction rate does not depend upon the superficial velocity with which the fluid stream is being flown into the reactor. Now, it should be noted that here the exponential dependence is exponential to the power of 1 by 2. So, therefore, the exponential dependence on temperature is not as strong as in the case of surface reaction limited situations.

So, therefore, we can see that the reaction rate in the case of internal diffusion limitations is 1 by dP and it depends exponentially on the temperature at which the reactor is being operated. So, next let us look at the surface reaction limited case.

(Refer Slide Time: 09:33)



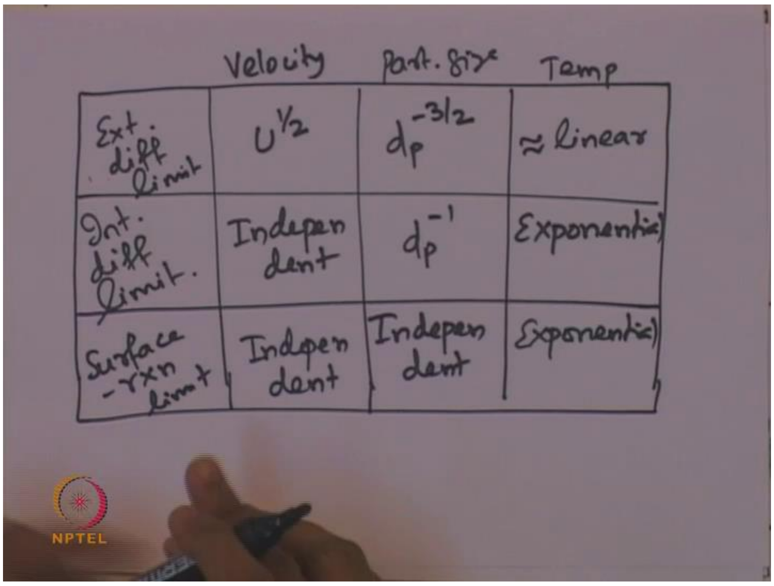
Surface - reaction limited

$-r_A' \rightarrow$ Indep. of particle size

$\rightarrow$ Strong function of T

So, in the surface reaction limited case the surface reaction limited case the reaction rate is now is independent of the size of the particle; it is independent of the particle size. And it is a strong function of the temperature at which the reactor is being operated. So, now if you put them altogether, if you put all of these 3 dependencies of the reaction rate on various systems parameters for all these 3 cases together. We can now form a table which captures the dependence of the reaction rate on various parameters.

(Refer Slide Time: 10:22)



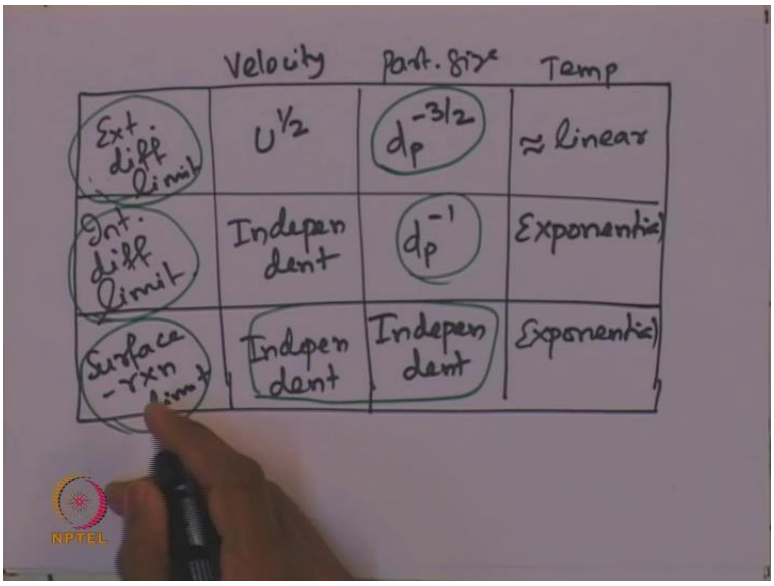
	Velocity	Part. size	Temp
Ext. diff limit	$U^{1/2}$	$d_p^{-3/2}$	≈ linear
Int. diff limit.	Indepen dent	d_p^{-1}	Exponential
Surface -rxn limit	Indepen dent	Indepen dent	Exponential

So, now let us draw a table. So, let us look at the external diffusion the case of external diffusional limitations. Under the external diffusional limitations what is its functional dependence on the velocity it is U to the power half. So, that is the functional dependence on velocity.

Then if a look at the particle size it depends upon dP to the power of minus 3 by 2 and then on temperature it is approximately linear. So, the reaction rate is approximately linear with respect to temperature in the external diffusional limitation case. Next, if you look at the internal diffusional case, diffusional limitations case the reaction rate is now independent of velocity; its independent of the velocity with which the fluid is being pumped into the reactor. And it is a function of dP to the power of minus 1 and it depends exponentially on the temperature; some exponential dependence on the temperature.

Now, if you look at the surface reaction case surface reaction limited case, then its independent of the velocity with which the fluid is being flown into the reactor; its independent of that. And it is also independent of the particle size and it has a strong exponential dependence on the temperature. So, therefore, if reaction is being performed the first step would be to perform the reaction at a certain velocity and different diameter of the particle.

(Refer Slide Time: 12:24)

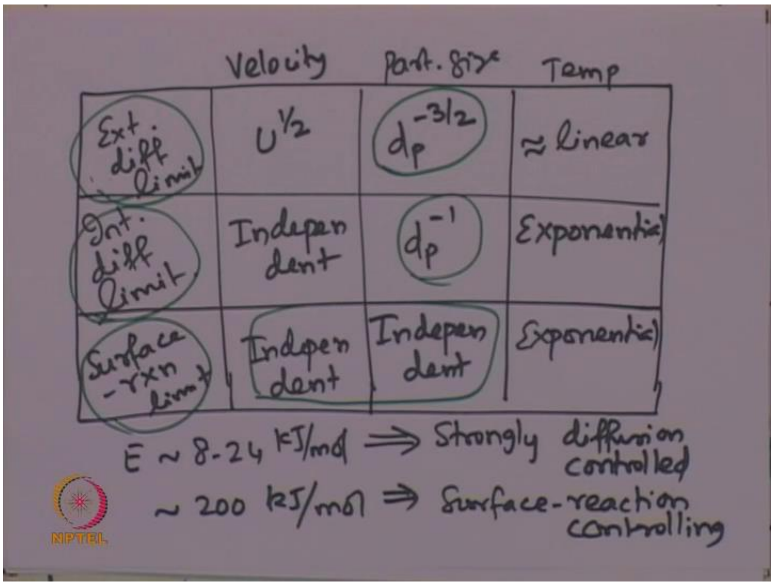


	Velocity	Part. size	Temp
Ext. diff limit	$U^{1/2}$	$d_p^{-3/2}$	≈ linear
Int. diff limit	Independent	d_p^{-1}	Exponential
Surface -rxn limit	Independent	Independent	Exponential

Now, if you look at the different diameter of the particle if the reaction rate by decreasing the particle size it correspondingly uses this expression of this shows this dependence of 1 by dP. Then it suggests that the particular reaction is under the internal diffusional limitations. Now, if it has a functional dependence of dP to the power of minus t by 2, then it suggests that is an exponentially external diffusion limited situations.

Now, if it is independent of the particle diameter if it is completely independent of the particle diameter then it the current condition suggests that experimental conditions are the essentially it is under the reaction surface reaction limited situation. So, as a rule of thumb if the activation energy is of the order of 8 to 24 Kilo Joules per mole, if that is the order of magnitude.

(Refer Slide Time: 13:01)



	Velocity	Part. size	Temp
Ext. diff limit	$U^{1/2}$	$d_p^{-3/2}$	≈ linear
Int. diff limit	Independent	d_p^{-1}	Exponential
Surface -rxn limit	Independent	Independent	Exponential

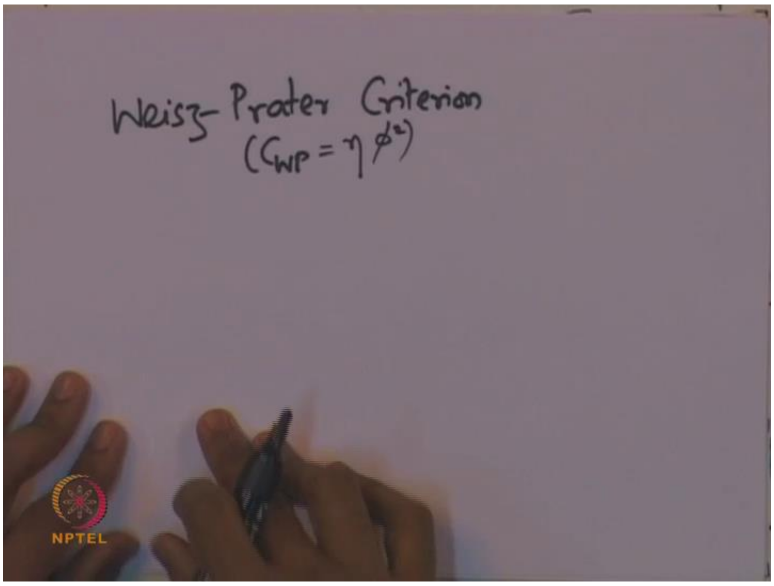
$E \sim 8\text{-}24$ kJ/mol ⇒ Strongly diffusion controlled

~ 200 kJ/mol ⇒ Surface-reaction controlling

Then it means that the reaction is actually strongly under strongly diffusional limitations strongly external diffusion controlled regime that is, external mass transport controlling it is under strong diffusion controlled digit. However, if it is about 200 kilo joules per mole then more often than, likely it will be a surface it will be a surface reaction controlled regime.

So, the reaction will be surface reaction controlling. So, this table summarizes the functional independence of various parameters. And how can an experiment be designing using these parameters in order to estimate whether the reaction is likely to be external diffusion limited or internal diffusion limited or the surface reaction limited.

(Refer Slide Time: 14:20)

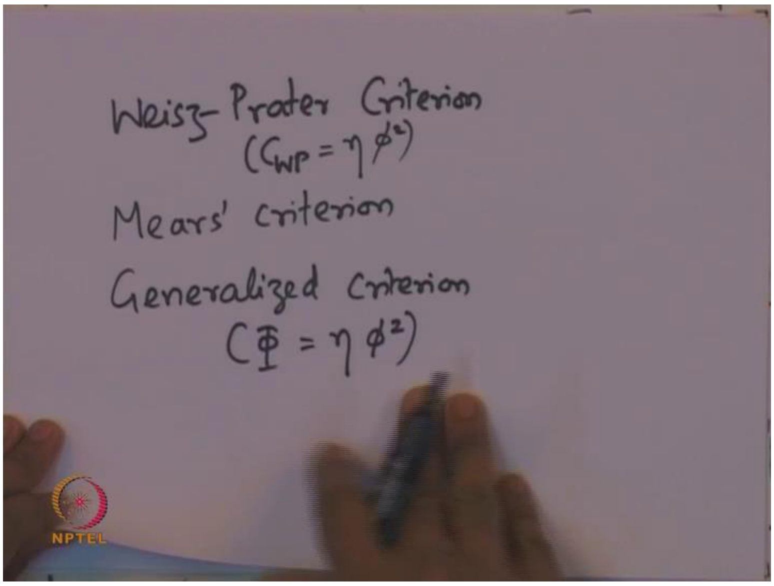


Weisz-Prater Criterion

($C_{WP} = \eta \phi^2$)

So, now, summarizing what we have learnt about various criteria is we have looked at the Weisz prater criterion. We have looked at Weisz prater criterion, it essentially uses a a parameter CWP which is equal to the effectiveness internal effectiveness factor multiplied by the corresponding Thiele modulus. This does not work and for all types of rate laws it works for a certain type of rate laws where the effectiveness factor Thiele modulus behavior is monotonic. And then we whether it is external diffusion controlled or not.

(Refer Slide Time: 14:53)



Weisz-Prater Criterion

($C_{WP} = \eta \phi^2$)

Mears' criterion

Generalized criterion

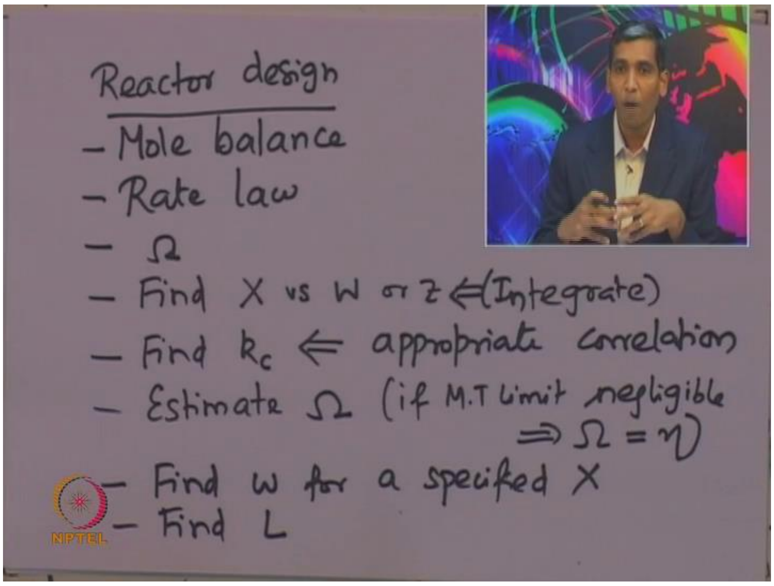
($C_{\Phi} = \eta \phi^2$)

And, then we looked at the generalized criterion where once again parameter capital phi which is equally to the overall effective which is equal to the local effectiveness or internal effectiveness factor for a any general any general and reaction mechanism multiplied by d Thiele modulus of that particular general mechanism. So, that particular product gives you a factor called capital phi which is used in which is used as a general criterion.

So, if phi is less than 1 then it is considered that the diffusional limitations does not exist and it is greater than 1, then the diffusional limitations strong diffusion limitations exist in the particular type of reaction. So, now, once we know how to identify whether the reaction is under the diffusion or the internal diffusional limitation or external diffusional limitation or surface reaction limited conditions. Then 1 may use this kind of information's such as the effectiveness factor into the reactor design.

So, the general algorithm to perform a reactor design; general algorithm to perform a reactor design is first 1 write some mole balance. A mole balance is written and then the law is identified the rate law is identify. And then based on the rate depending upon the experimental data 1 may be able to find out whether it is external diffusion controlled or internal diffusion controlled. So, based on that we can find out what is the expression for the overall effectiveness factor which incorporates all types of limitations.

(Refer Slide Time: 16:47)



Reactor design

- Mole balance
- Rate law
- Ω
- Find X vs W or $z \Leftarrow$ (Integrate)
- Find $k_c \Leftarrow$ appropriate correlation
- Estimate Ω (if M.T limit negligible $\Rightarrow \Omega = \eta$)
- Find W for a specified X
- Find L

Then find the by solving the mole balance you can use this overall effectiveness factor and you can find out what is the rate law based on the observable quantities such as, the bulk concentration. And, then we can find what is the relationship between the conversion X by taking stoichiometry into account versus the weight of the catalyst which may be used for conducting the reaction to attain a certain conversion or the position inside the reactor? Then following which can be obtained by integration of the mole balanced.

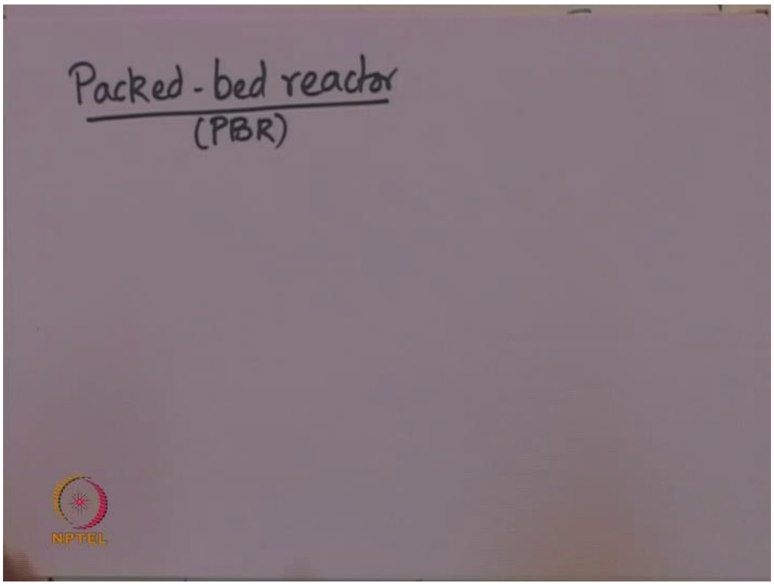
So, integrate the mole balance and 1 can get the relationship between x and the weight of the catalyst or the position inside the catalyst. Now, the position at which the desired exit conversion can be achieved is what does the length of the reactor that needs to be designed or that is the required length of the reactor for attaining a certain conversion. Then the next step is to find the mass transport coefficient kc, this can be obtained using various correlation. So, 1 may use the appropriate correlations.

Now, if it is not external mass transport controlled, then the mass transport coefficient really does not play much role here. So, in that case this step can be ignored and the effectiveness factors will simply be equal to the internal effectiveness factor. So, the overall effectiveness factor will be equal to internal effectiveness factor.

So, then the next step is to estimate based on the various properties and the parameters and next step is to estimate the overall effectiveness factor. If mass transport, mass transport limitations are negligible then the overall effectiveness factor is approximately equal to the internal effectiveness factor.

Then next step is to find the weight of the catalyst for a specified conversion and then find the length of the reactor. So, this is the general recipe for performing a reactor design in order to obtain the design parameters such as, how much weight of catalysts is required to obtain a certain conversion what should be the length of the reactor to obtain the desired conversion. So, now, let us look at little bit more details of packed bed reactor and the design of packed bed reactors.

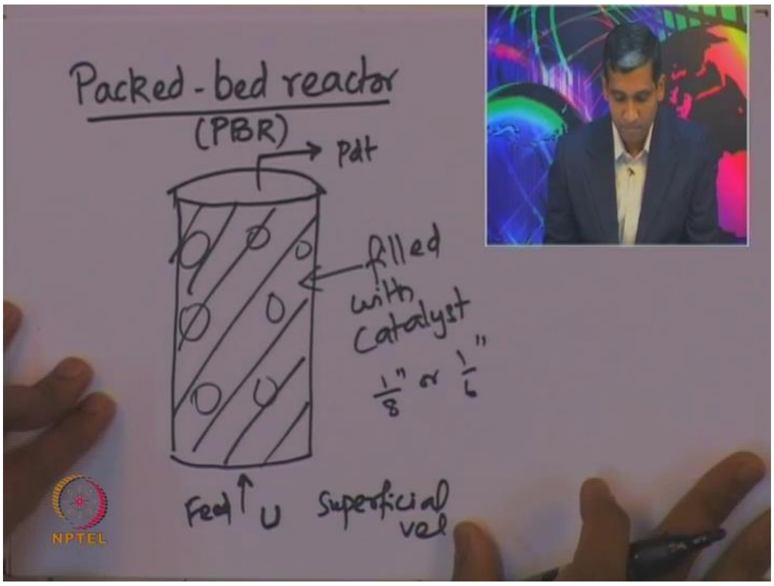
(Refer Slide Time: 19:35)



Packed - bed reactor
(PBR)

The packed bed reactor here after will simply be referred to as PBR which stands for packed bed reactor. So, packed bed reactor is essentially a tube which is filled with catalyst inside and the reactants are flown from 1 end and the gas stream the reactant species present in the gas stream they go into the catalyst and then get adsorbed onto the site of the catalyst. And the reaction occurs and soon after the reaction occurs the product leaves the catalyst and then moves into the gas stream and the product leaves the reactor. So, it is essentially a tube.

(Refer Slide Time: 20:30)

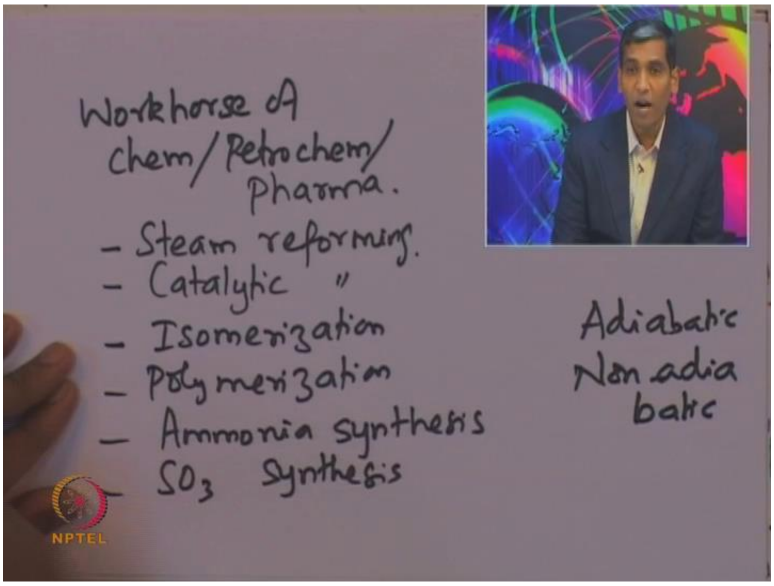


Packed - bed reactor
(PBR)

It is a tube which is filled with catalyst filled with catalyst pellet. So, these are catalyst pellets. So, the catalyst pellets may be spherical it may be small cylindrical there are various types of shapes that may be used depending upon the nature of the reaction that is being conducted. And the typical size of the catalyst if it is a spherical particle or the approximate hydraulic radius would be about 1 8-th inch or 1 6-th inch. That is a typical size of the catalyst that is actually being used inside a commercial packed bed reactor.

Now, the fluid stream may be flowing from the bottom of the reactor with let us with the velocity superficial velocity of U. So, that is the superficial velocity and the product comes out from the top. So, this is where the product comes out the feed goes here the feed stream goes in from here and then the product comes out from the top. So, it may be that there may be different kinds of reactions that can be conducted inside such a packed bed reactor. So, a packed bed reactor is actually the workhorse of chemical, petrochemical and pharmaceutical industries.

(Refer Slide Time: 21:45)



Workhorse of
chem/Petrochem/
Pharma.
- Steam reforming.
- Catalytic "
- Isomerization
- Polymerization
- Ammonia synthesis
- SO_3 synthesis

Adiabatic
Non adiabatic

So, it is the workhorse of chemical, petrochemicals and pharmaceutical industries slash pharma industries. It is used in many different processes conversion of many different chemicals and a good example of that will be steam reforming; its 1 of many good examples of situation where packed bed reactor is used. And then its use far catalytic reforming process, it is used in isomerization process, it is used in polymerization process and it is used in ammonia synthesis.

These are some of the examples where packed bed reactor is routinely being used in industrial conditions, industrial settings, ammonia synthesis. It is also used in SO3 synthesis. So, these are some of the examples of situations where packed bed reactor is being used in reality. And the packed bed reactor can in principle be operated under 2 more, 1 can be operated under adiabatic mode or a non adiabatic mode.

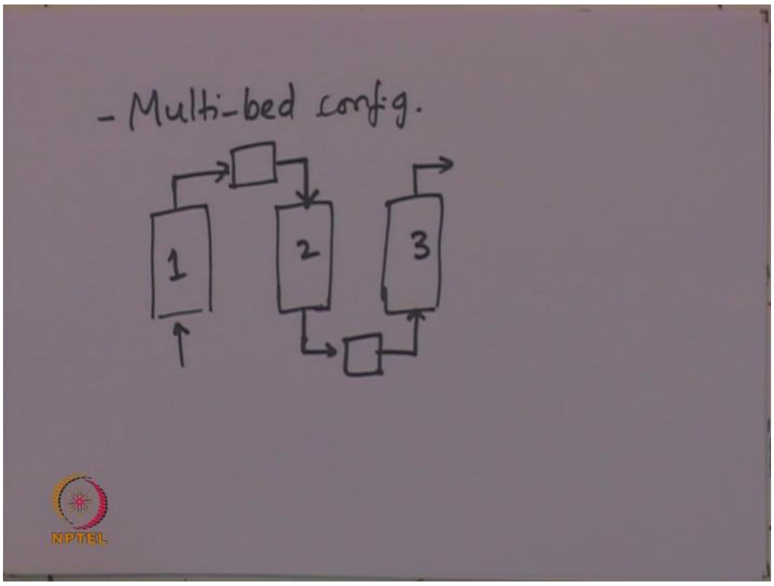
So, adiabatic mode is a situation where no heat that is actually lost from the reactor to the external sounding. So, that is called an adiabatic situation. Another configuration is an non adiabatic situation where the reactor may not be conducted at an adiabatic conditions. The actor maybe it is an maybe it is an exothermic reaction where there is a cooling fluid which is flowing in the jacket and it might be the removing the heat that is being generated because of the exothermicity of the reaction.

Now, this is required this may be required under many situations because if there is an exothermic reaction, then the local temperature inside the reactor can actually increase. And that may lead to if it crosses the making point of the catalyst then it may lead to melting of the catalyst. Or if it is present close to the walls and it is a if it is an undesirable temperature then it poses a very serious safety concern.

So, therefore, it is very important to manage the heat inside the reactor. And so, a fluid is being circulated around constantly the heat is being removed, if it is an exothermic reaction which generates heat due to the reaction. So, there are gently 2 modes of operating 1 is the adiabatic where there is no heat is removed from the reactor; where the exterior of the tubular reactor is insulated.

Then, other situation: where it is a non adiabatic situation; where the heat maybe removed from the exterior wall of the tubular reactor. Now, the packed bed reactor also is being operated under different configuration.

(Refer Slide Time: 24:50)



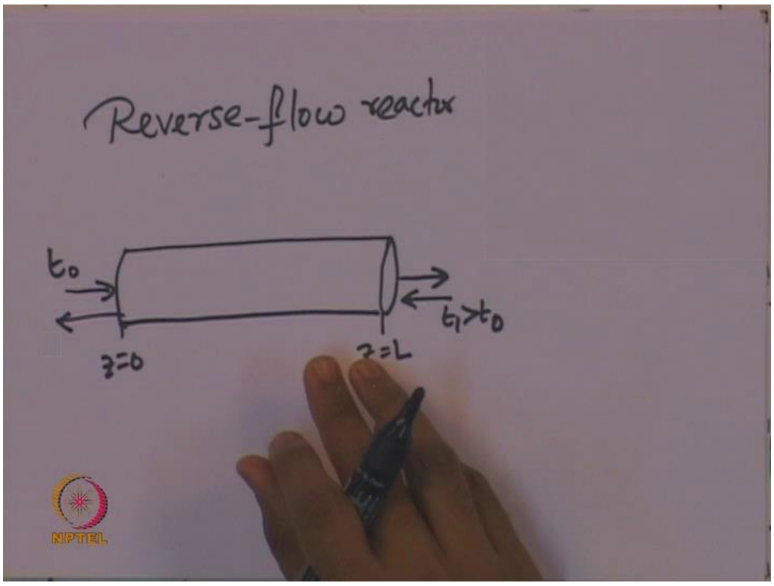
They are several configurations that have being a used in the in the industry and some of these are multi bed reactor. So, multi bed configuration in a multi bed configuration, there are multiple beds which are present as multiple tubular reactors.

Multiple tubular reactors, where the fluid stream goes into 1 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 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 etcetera. 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; that means, the reaction is conducted is different.

So, therefore, 1 may actually pack different catalyst in each of these multiple bed. And so that way a desired conclusion can be achieved and as well the catalyst deactivation can be prevented.

(Refer Slide Time: 26:18)



So, in 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 flown let us say this is at z equal to 0.

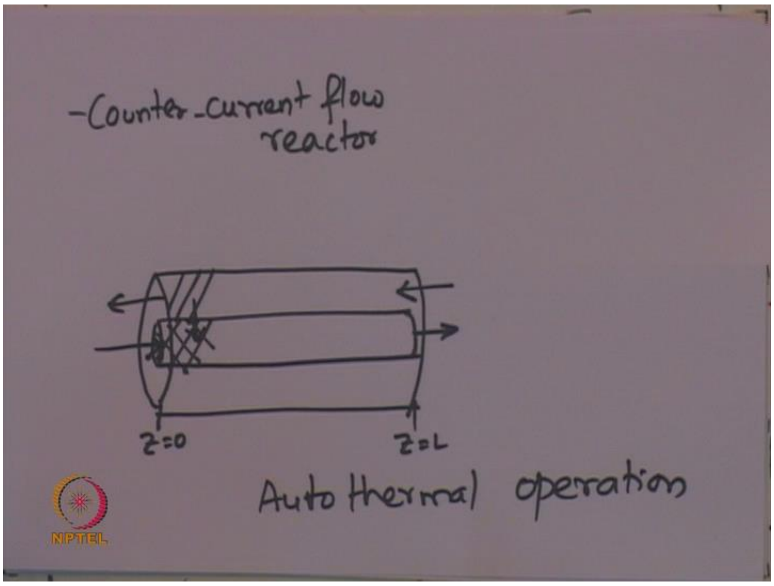
So, this is the entry point at certain time and this is z equal to l. So, at a certain time the fluid enters the reactor at z equal to 0 and then it leaves the reactor at z equal to L. At a later time t 1 let us say if this is t 0 at a later time t 1 which is greater than t 0 the fluid is now entering from into the actor from the from z equal to L. And it flows in the reverse direction and then leaves the reactor at z equal to 0.

So, this is at time t equal to t 1. So, this kind of 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 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 template is likely to increase significantly.

Now, in order to and that may actually deactivated the catalyst or it man lipose some serious safety problems. In order to prevent that at a certain preset frequencies if the fluid stream is now the directional the fluid team 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 byproduct the there are most part of the actor will not be exposed to a certain a very high temperatures and this can actually prevent the deactivation of the catalyst.

This provides a very useful mechanism to protect the a catalyst which is very expensive. So, this is a very well known configuration and the other configuration which is also a fairly used particularly if you want to if the reactant feed stream is lean concentration. If the concentration of the reactant is very small in the feed then a countercurrent flow reactor is being used.

(Refer Slide Time: 28:48)

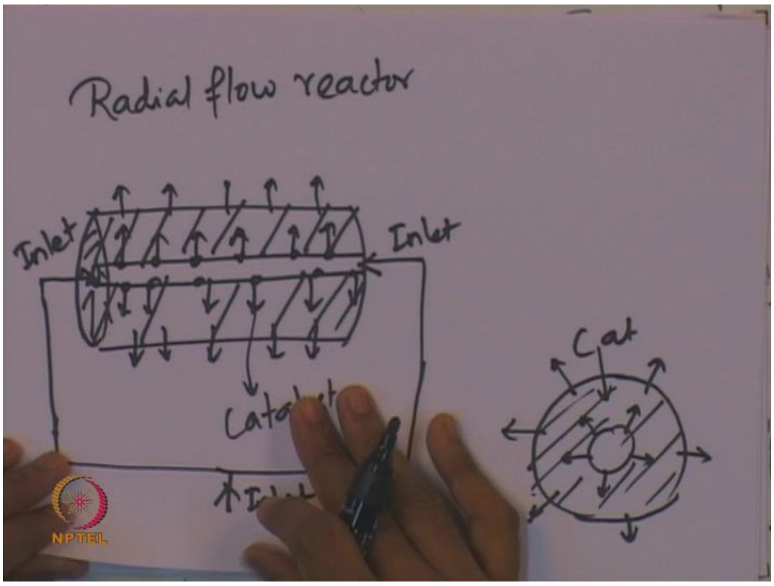


So, a countercurrent flow reactor is essentially a 2 chamber reactor. So, it will be 2 concentric cylinders 2 concentric cylinders. Now, in this concentric cylinder the feed stream is flown in 1 direction in 1 chamber and in the other direction in the other chamber. So, the fluid stream is now flown at a in a countercurrent fashion where the fluid stream in the inside tube leaves enters the reactor at z equal to 0 and leaves that the reactor z equal to L. While the fluid stream in the outside concentric cylinder external cylinder enters at z equal to L and leave at z equal to 0.

So, this has an 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 date 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 flow then the feet stream which is present near the inlet of the reactor in the in the inside tube, can actually obtain heat from the fluid stream which leaves the reactor from the outside chamber.

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 leave the reactor. So, in order in order not to lose the heat that it has 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 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 is yet the desired conversion is required.

(Refer Slide Time: 31:31)



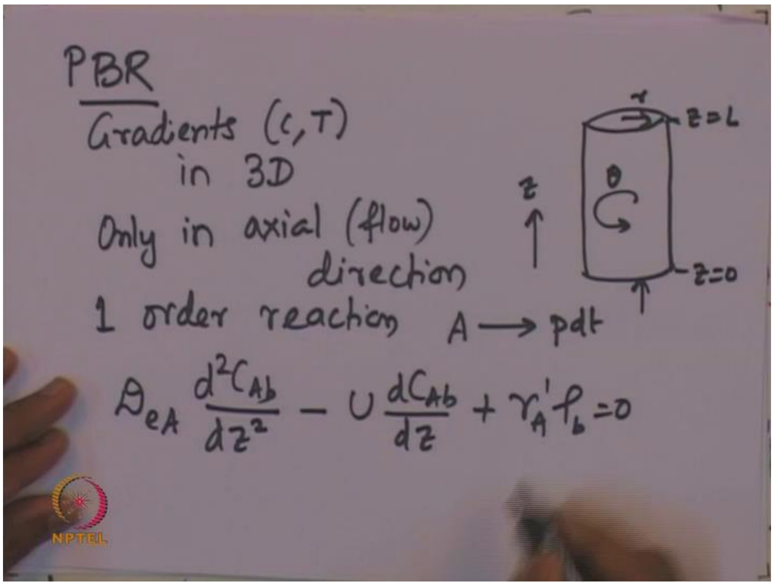
In yet another configuration which is also being used in industry is called the radial flow reactor. So, in a radial flow reactor what happens is suppose if this is the tube and there is a small concentric channel which is present inside the reactor. And the space between the concentric channel inside and the exterior of this tube is actually filled with catalyst.

Now, the fluid stream which is fluid stream containing that reactant is made to flow through the inside chamber from both sites. The fluid stream flow simultaneously from both sides its inlet fluid stream. Now, when it flows from both sites a sparger is kept along the periphery of the inside you these are tiny holes which are placed at the certain precalculated distance. And s o, the fluid stream which enters through the reactor on either sides they leave they go into the chamber which contains the catalyst particle through this sparger.

So, the feed stream is parsed uniformly in all directions inside the radial flow reactor and the reaction happens in the catalyst and then the fruits team leaves from the curved surface of this exterior tube. So, this is what is called as a radial flow reactor a side view of this reactor it looks like this. So, if I take a cross section of the 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 their catalyst is present here.

So, that is the catalyst and the action happens in the in the region where the catalyst is packed and then the fluid stream leaves from the exterior of this of this chamber. So, this kind of an operation is what is called as a radio 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.

(Refer Slide Time: 34:08)



PBR

Gradients (c, T)
in 3D
Only in axial (flow) direction
1 order reaction A → pdt

$$D_{eA} \frac{d^2C_{Ab}}{dz^2} - U \frac{dC_{Ab}}{dz} + r_A' \rho_b = 0$$

So, let us look at the a design of packed bed reactor. Let us look at a packed bed reactor design. Now, the in a tubular reactor a packed bed is initially 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 reduction. And then it is also expected the gradients are expected to be present in both the radial direction and the angular direction.

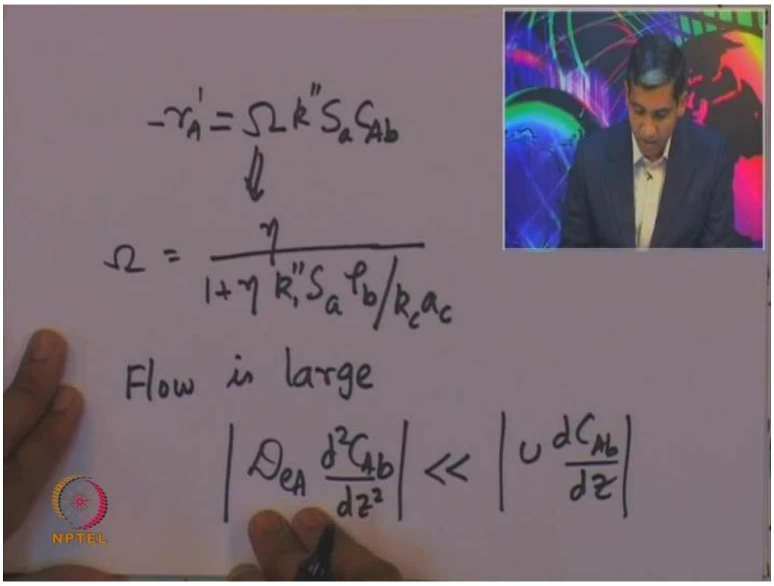
So, the in principle the temperature and concentration gradients are expected to be present in all 3 dimensions. And it is only concentration gradient if the reactors operator and isothermal conditions. So, therefore, the gradients concentration and temperature in all 3 dimensions, it is present in all 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 1 of the lectures before. So, if the 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 is the axial dispersion coefficient multiplied by d square CAB which is the concentration of the species in bulk divided by Dz square. That is the, that captures the diffusion of species in the reactor in the axial direction.

So, minus U into dCAB by dz plus rA prime into rho d equal to 0. Now for ... So, let us draw the coordinates. So, if suppose if this is the tubular reactor if 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 theta. So, theta is the angular direction. So, there are no gradients we assume that there are no gradients in the theta 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 equal to 0 z equal to l. So, the gradients are the first term here corresponds to the diffusion in the 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 is being consumed to form the necessary product.

(Refer Slide Time: 37:17)



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

$$\Downarrow$$

$$\Omega = \frac{\eta}{1+\eta k_1'' S_a \rho_b / k_c a_c}$$

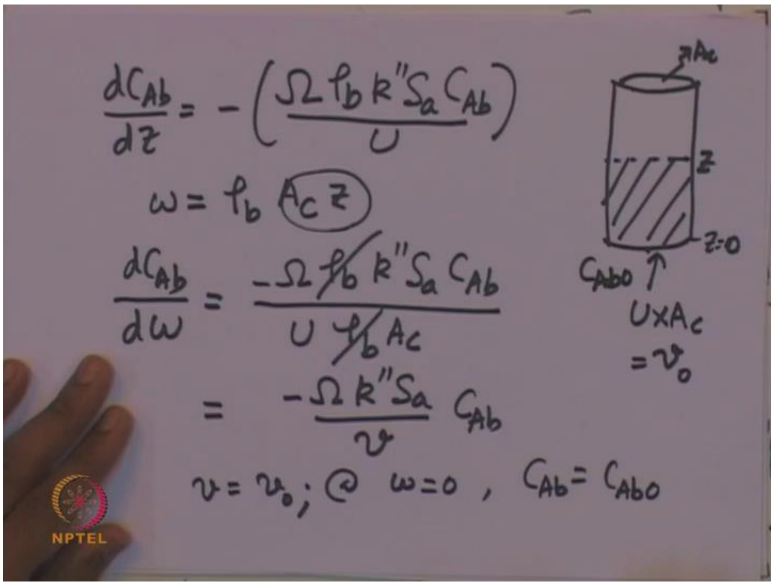
Flow is large

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

So, suppose if the if we know the overall effectiveness factor, then we can write the reaction rate as minus rA minus rA 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 CAB. Now, for the first order reaction the overall effectiveness factor is given by the local effectiveness factor eta divided by 1 plus eta into the first order reaction constant k of double prime 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 quantities such as the bulk concentration of the species which is which is reacting to form the necessary products. So, now, we can suppose if we assume that the flow through the bed this significant if the flow is large 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.

(Refer Slide Time: 38:17)



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

$$\omega = \rho_b \boxed{A_c z}$$

$$\frac{dC_{Ab}}{d\omega} = \frac{-\Omega \cancel{\rho_b} k'' S_a C_{Ab}}{U \cancel{\rho_b} A_c}$$

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

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

$$U \times A_c = v_0$$

So, under this condition we can actually we can rewrite the mole balance as dCA by dCA bulk by dz. That is equal to minus omega into rho d which is the bulk density of the catalyst into k double prime into Sa into CAB divided by U. Now, sometimes the design parameter that 1 needs to estimate may be the weight of the catalyst or in sometimes it may be the it may be the size of the reactor given in a certain conversion. So, therefore, we can actually convert this equation in terms of the weight of the catalyst.

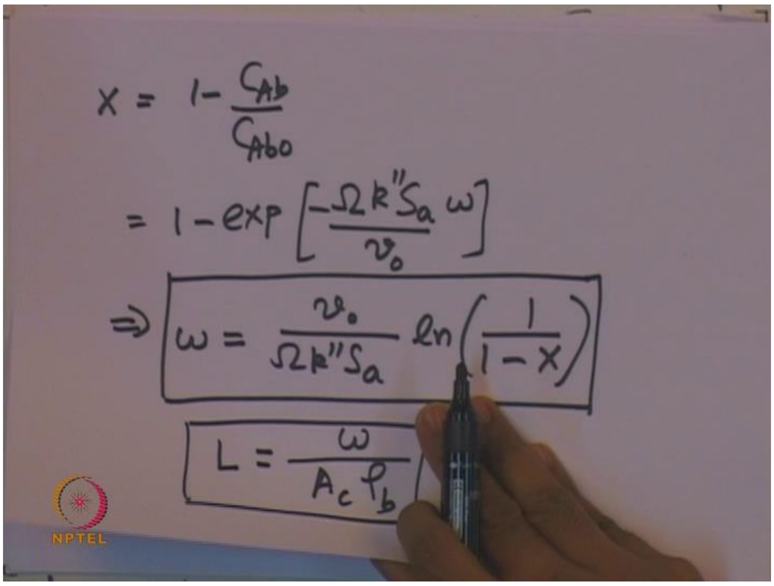
So, the weight of the catalyst that is packed till a certain a location in the action direction is given by the bulk density of the catalyst multiplied by the cross sectional area of the reactor multiplied by the corresponding position. So, if this is the tubular reactor and let us says we are looking at this particular z z and if the cross sectional area is AC cross sectional area of the reactor is AC. Then we want to know, what is the total amount of weight of catalyst that is packed from z equal to 0 to up to some particular point z?

So, that is given by rho 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 dCAB by dw that is equal to minus overall effectiveness factor into rho b into k double prime Sa CAB divided by u into rho b into AC. So, that is because of the dependence of this weight of the catalyst on the density and the cross sectional and that is why we get these 2 terms here.

So, you can cancel out these 2 and u into AC, if u is the superficial velocity with which the fluid is entering the reactor u into the ac which is the cross sectional will give you the volumetric flow rate with which the fluid stream is entering the reactor. So, therefore, this can be written as minus overall effectiveness factor into Sa divided by the volumetric flow rate CAB. So, the volumetric flow rate at the inlet could be v naught and the volumetric flow rate at that particular location if there is. So, 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 is equal to v naught. And if, and also if we assume that at and if you assume that at if they weight of the catalyst is 0 then the CAB which is the bulk concentration that is equal to the concentration with which the fluid actually is entering the reactor. So, CAB 0 is the concentration with which the fluid is actually entering the packed bed reactor in which the reaction has happened.

(Refer Slide Time: 41:50)



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

$$= 1 - \exp\left[\frac{-\Omega k'' S_a \omega}{v_o}\right]$$

$$\Rightarrow \boxed{\omega = \frac{v_o}{\Omega k'' S_a} \ln\left(\frac{1}{1-X}\right)}$$

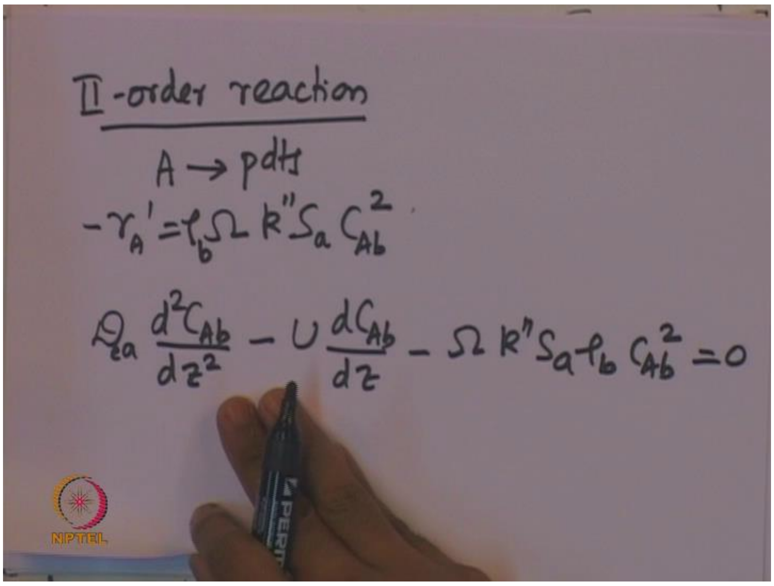
$$\boxed{L = \frac{\omega}{A_c \rho_b}}$$

This equation can now be integrated to find that the conversion x is given by 1 minus CAB by CAB naught and that is equal to 1 minus exponential of minus omega. Which is the overall effectiveness factor multiplied by k double prime multiplied by the surface area of the catalyst available for the reaction per unit gram of catalyst multiplied by w divided by volumetric flow rate v naught with which the fluid is actually entering the reactor. Or we can rewrite this as w equal v naught divided by omega k double prime Sa into lon of 1 by 1 minus 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 into density.

So, this method a mechanism, this design provides the mechanism by which for a specified conversion if the assumption that the bulk flow is significantly larger than that of the a diffusion. Then we can actually find out what is the weight of the catalyst which is require for a given conversion and what is the length on the reactor for a specify conversion.

(Refer Slide Time: 43:40)



II-order reaction

$A \rightarrow pdts$

$-r_A' = \rho_b \Omega k'' S_a C_{Ab}^2$

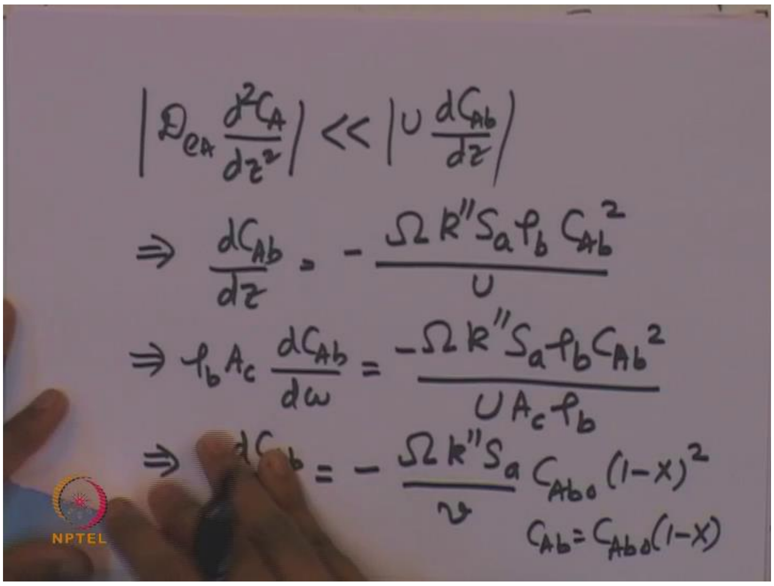
$$D_{ea} \frac{d^2 C_{Ab}}{dz^2} - U \frac{dC_{Ab}}{dz} - \Omega k'' S_a \rho_b C_{Ab}^2 = 0$$

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 products is the reaction scheme and if minus rA prime is the rate at which the species a is being consumed.

If that is given by the overall effectiveness factor omega multiplied by the corresponding specific rate constant k double prime into the surface area of the catalyst per unit weight of the catalyst into CAB 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 into d square CAB by dz square. That is the diffusion term which with the rate at which the species is defusing inside the reactor and minus u times dCAB by d z minus omega into k prime into Sa into rho b into CAB square. So, it should be a rho b here.

So, the that is 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 in other parameters of the system including the specific rate constant. So, now, we can solve this if we assume once again that the bulk flow is significantly larger than the corresponding diffusion rate.

(Refer Slide Time: 45:05)



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

$$\Rightarrow \frac{dC_{Ab}}{dz} = -\frac{\Omega k'' S_a \rho_b C_{Ab}^2}{u}$$

$$\Rightarrow \rho_b A_c \frac{dC_{Ab}}{dw} = \frac{-\Omega k'' S_a \rho_b C_{Ab}^2}{u A_c \rho_b}$$

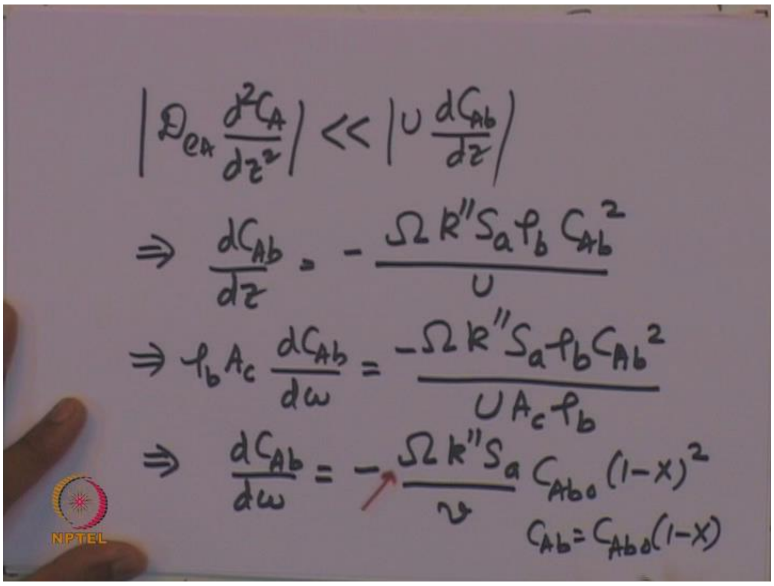
$$\Rightarrow dC_{\ b} = -\frac{\Omega k'' S_a}{\upsilon} C_{Ab0}(1-x)^2$$

$$C_{Ab} = C_{Ab0}(1-X)$$

Then the Da quare is significantly smaller to the corresponding bulk flow. Then the mole balance will simply be reduced to DCA bulk buy dz. That is equal to minus overall effectiveness factor omega multiplied by k doubles prime into Sa into rho b into CAB 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 AC into dCAB by dw which is the where w stands for the weight of the catalyst.

That is equal to minus omega CAB square divided by u into AC into rho b, that is the bulk density of the catalyst. And so, from here you can find that dCAB by dw that should be equal to minus omega k double prime Sa divided by the volumetric flow rate v multiplied by CAB 0 into 1 minus x the whole square. So, this expression provides a relationship between the concentration of the species and other parameters and where, CAB is equal to CAB 0 into 1 minus x where x is the corresponding conversion. So, now we can also incorporate the relationship between the concentration and conversion on the left hand side of the expression.

(Refer Slide Time: 47:00)



$$\left|\mathcal{D}_{eA}\frac{d^2C_A}{dz^2}\right| << \left|u\frac{dC_{Ab}}{dz}\right|$$

$$\Rightarrow \frac{dC_{Ab}}{dz} = -\frac{\Omega k'' S_a \rho_b C_{Ab}^2}{u}$$

$$\Rightarrow \rho_b A_c \frac{dC_{Ab}}{dw} = \frac{-\Omega k'' S_a \rho_b C_{Ab}^2}{u A_c \rho_b}$$

$$\Rightarrow \frac{dC_{Ab}}{dw} = -\frac{\Omega k'' S_a}{v} C_{Ab0}(1-x)^2$$

$$C_{Ab} = C_{Ab0}(1-x)$$

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 equal to 0 the weight of the catalyst is is 0. That is there are no catalyst 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 used such kind of a design can be performed for rate law which is a non monotonic that is it is a non n-th order type reaction. 1 could actually write a design equation for adsorption inhibition type reactions for a Langmuir Hinshelwood type reaction. And such kind of a reaction 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.