Chemical Reaction Engineering - II
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Module - 6
Lecture – 28
Packed-bed Reactor Design: External Mass Transfer Limitations

In the last lecture we looked at mass transport along with reaction in a single catalyst pellet. We quantified the simultaneous mass transport for species from bulk to the surface of the catalyst, while the reaction is actually simultaneously happening in the catalyst. We also saw that there is a mass transport limited regime and there is a surface reaction regime and that can be controlled by the rate at which the velocity, superficial velocity with which the fluid is actually flowing through the reactor or around the catalyst pellet for a fixed value of the particle diameter.

We can also look at fixing the superficial velocity and changing the particle diameter. But having a very tiny particle, which will actually, may guarantee surface reaction limitations, is actually, may not be a desirable situation because it will increase the pressure drop. Now, when we talk about pressure drop, we really are looking at what is the rate at which the fluid is actually flowing through the entire reactor.

So, we will need to next look at how to actually extend this design at a single particle or single catalyst level, where we looked at the boundary layer around a single particle and we can extend that to a packed-bed reactor. So, let us look at how a packed-bed reactor will look like.

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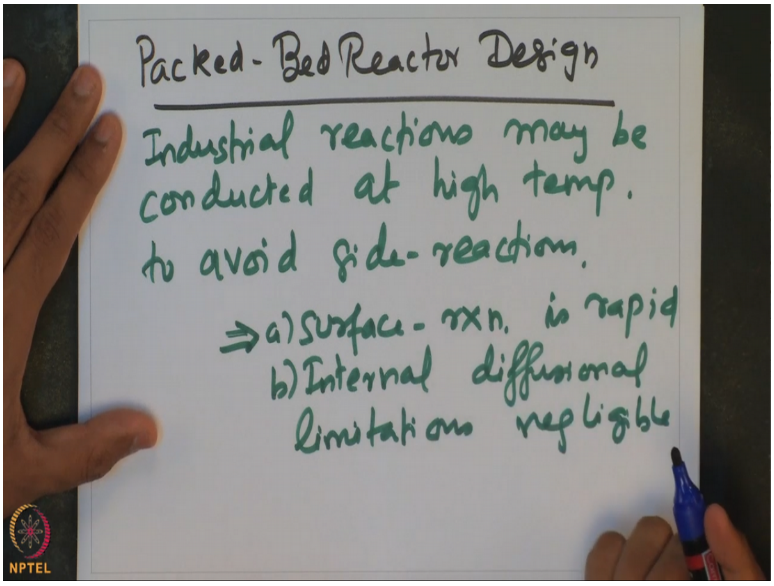

Packed-Bed Reactor Design

Industrial reactions may be conducted at high temp. to avoid side-reaction.

⇒ a) surface-rxn. is rapid
b) Internal diffusional limitations negligible

So typically, the industrial reactions may be conducted at high temperatures, particularly to avoid. So therefore, if the reaction is conducted at high temperature, we can assume that the surface reaction is rapid. And we can also assume that the internal diffusional limitations are negligible. In fact, in one of the future lectures, we will actually see how to combine both the internal diffusional limitations and the external diffusional limitations in one of the future lectures. So, what are the design parameters of a packed-bed reactor?

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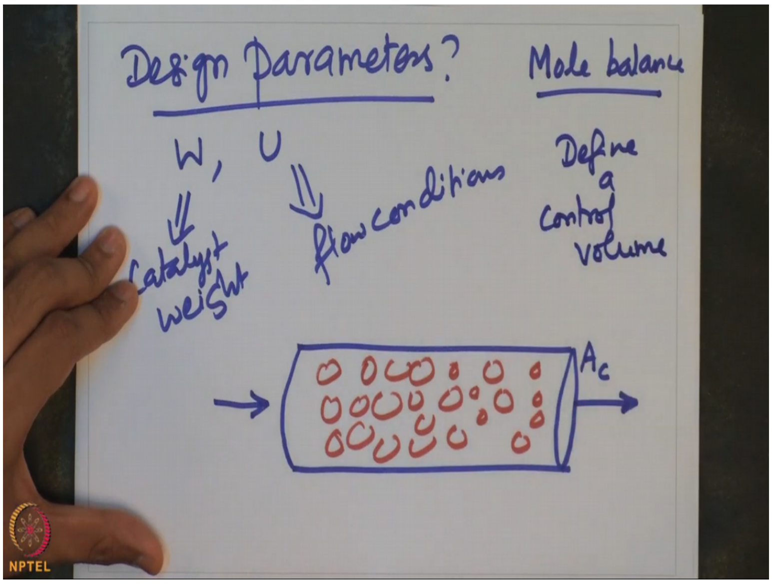

Design Parameters?

W, U

$\Downarrow$ Catalyst weight

$\Downarrow$ flow conditions

Mole balance

Define a control volume

What are the design parameters? The design parameters are essentially the flow conditions and the weight of the catalyst. Recall that the catalyst is actually very expensive. So, conducting a reaction in a packed-bed reactor would actually require having as minimum weight of the catalyst as possible. Because catalyst is the most expensive component in most of the cases. And so, weight of the catalyst is actually an important parameter.

And of course, the operating condition which is basically the rate at which the fluid has to be flown and so on and so forth. So, essentially the catalyst weight and the flow conditions. These 2 are actually an important parameter. So, let us look at how a packed-bed, let us try to sketch a packed-bed reactor. So, let us say that the, it is filled with catalyst. And let us assume that the cross-sectional area of the reactor is A c.

And the fluid is actually flowing through the reactor. Let us say that this is the entry to the reactor and this is the exit of the reactor where the fluid steam is actually leaving the reactor.

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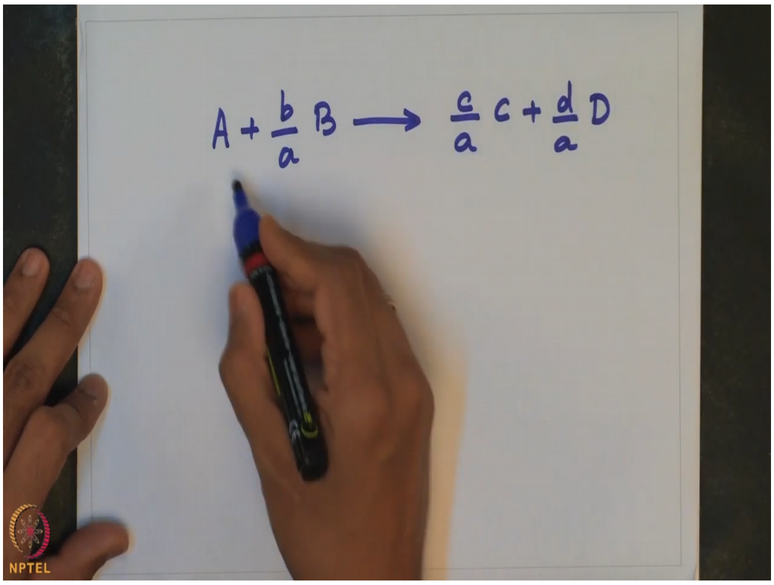

That is the stoichiometric equation that we actually used for designing this particular packed-bed reactor design. Now, we can write a mole balance in order to quantify the process that is happening in a packed-bed reactor. Now, what is the first step in writing a mole balance? We need to define a control volume. But, before we define a control volume, we need to specify what is the positive direction and the coordinates of the reactor. So, let us look at that for a moment.

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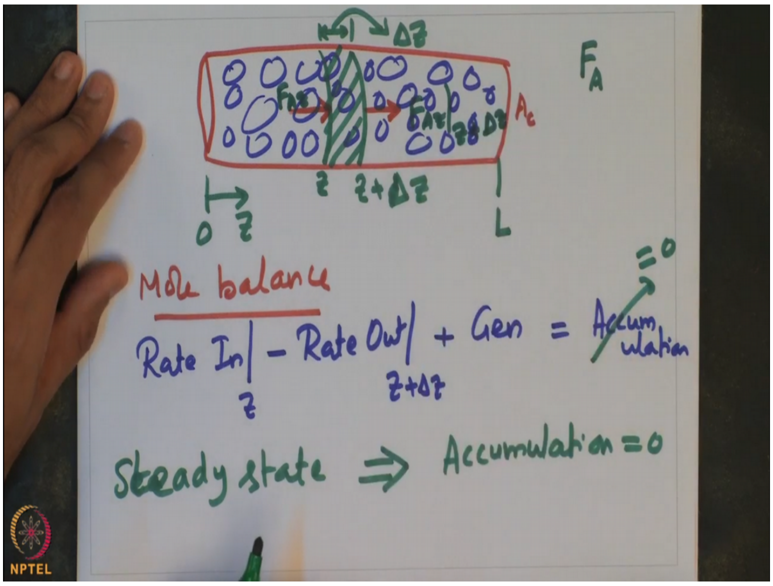

Mole balance

$$\text{Rate In}\Big|_{z} - \text{Rate Out}\Big|_{z+\Delta z} + \text{Gen} = \cancel{\text{Accumulation}}$$

$$\text{Steady state} \Rightarrow \text{Accumulation} = 0$$

So, we have a reactor whose cross-sectional area is A, A c. And we have catalyst filled with, we have catalyst filled inside; reactor is packed with catalyst. So, let us define a small element. And if this is my, Z is my positive direction, going from 0 to, let us say L. L is the length of the reactor, cylindrical reactor. And let us say that this location is some Z. And if this width is let us say delta Z. And so, this location is essentially given by Z + delta Z.

Now, how do we write a mole balance? What are the things we need to define? We need to define what is the rate at which, molar rate at which the species is actually entering this element Z and what is the molar rate at which the species is actually leaving that particular location. So, what is the balance, what is the mole balance? The mole balances is the rate at which the species is entering at Z – the rate at which the species is living at Z + delta Z + whatever is generated in that control volume, that should be = accumulation.

So, this is the mole balance. And suppose if we assume steady-state, which means that accumulation is 0. So, this term essentially cancels out. And now, what is the rate at which the species is coming in? Suppose, let us say that F A is the molar rate and F A Z is the rate at which the species comes into this element at Z. And F A Z at Z + delta Z is the rate at which the species actually leaves from that element. So, the rate in, is essentially =; So, let us now spell it out.

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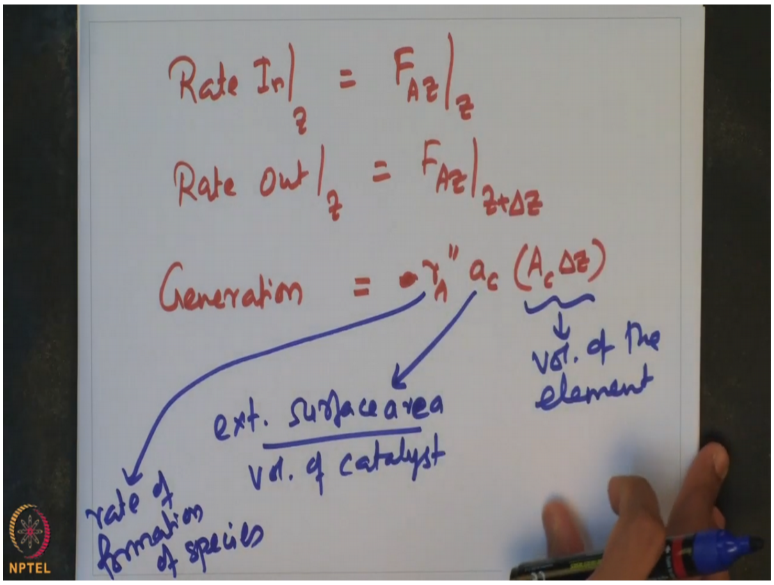

$$\text{Rate In}\Big|_z = F_{Az}\Big|_z$$

$$\text{Rate Out}\Big|_z = F_{Az}\Big|_{z+\Delta z}$$

$$\text{Generation} = r_A'' \, a_c \, \underbrace{(A_c \Delta z)}_{\text{vol. of the element}}$$

rate of formation of species

$$\frac{\text{ext. surface area}}{\text{vol. of catalyst}}$$

So, rate in at Z is = F A Z at Z. F A Z is the molar rate at which the species actually enters the element. And the rate out at Z is = F A Z at Z + delta Z. Now, what is the generation term? The generation term is = r A double prime. That is the rate at which the species is actually formed. That multiplied by the catalyst exterior surface area per unit volume of the catalyst, multiplied by A c into delta Z.

This is the volume of the element. And this is the exterior surface area per volume of catalyst. And this is the rate of formation of species. So, we have all the 3 quantities that we need. So, we can now plug this into the mole balance. So, what is the mole balance. The mole balance is the rate at which species comes into the element;

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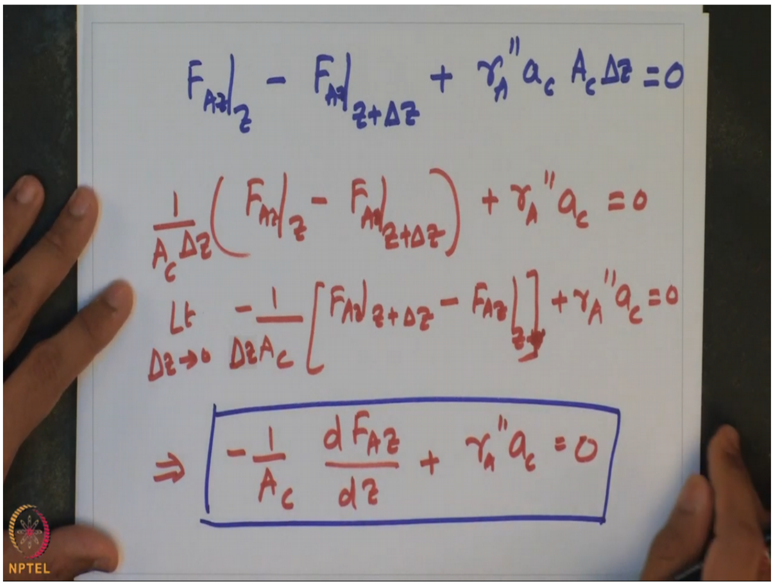

$$F_{Az}\Big|_z - F_{Az}\Big|_{z+\Delta z} + r_A'' a_c A_c \Delta z = 0$$

$$\frac{1}{A_c \Delta z}\left(F_{Az}\Big|_z - F_{Az}\Big|_{z+\Delta z}\right) + r_A'' a_c = 0$$

$$\underset{\Delta z \to 0}{Lt} \; -\frac{1}{\Delta z A_c}\left[F_{Az}\Big|_{z+\Delta z} - F_{Az}\Big|_z\right] + r_A'' a_c = 0$$

$$\Rightarrow \boxed{-\frac{1}{A_c}\frac{dF_{Az}}{dz} + r_A'' a_c = 0}$$

Which is F A at Z – F A at Z + delta Z. That is the rate at which species leaves the element, + r A double prime into exterior surface area of the catalyst per unit volume of the catalyst, multiplied by A c into delta Z. That is the volume of the element. And that should be = 0 because accumulation is 0. So, now, we divide this expression by A C and delta Z. So, we can see that this can be written as, 1 by A c into delta Z + r A double prime into a c = 0.

So, if I put, impose the condition that limit delta Z goes to 0. That is, if it is a small element. Then I can rewrite these expression as, limit as delta Z goes 0 – 1 by A c into F A Z + delta Z – F A Z. This is the F A Z which is the rate at which the species is actually flowing in the Z direction + r A double prime into a c = 0. What is this expression? This is nothing but the first differential of the rate with respect to Z.

So, that is = – 1 by A c d F A Z divided by d Z + r A double prime into a c = 0. So, this is the mole balance for the packed-bed reactor. So, this expression gives the mole balance corresponding to the packed-bed reactor. We have assumed that all processes are actually 1 dimensional. We assume that the concentration of the species in the cross-section is actually uniform, which means that the gradients are negligibly in the negligible in the cross-section of the reactor.

How do we find this rate now, F A Z. The rate at which the species has actually diffusing, the molar rate of the species at any location is essentially given by;

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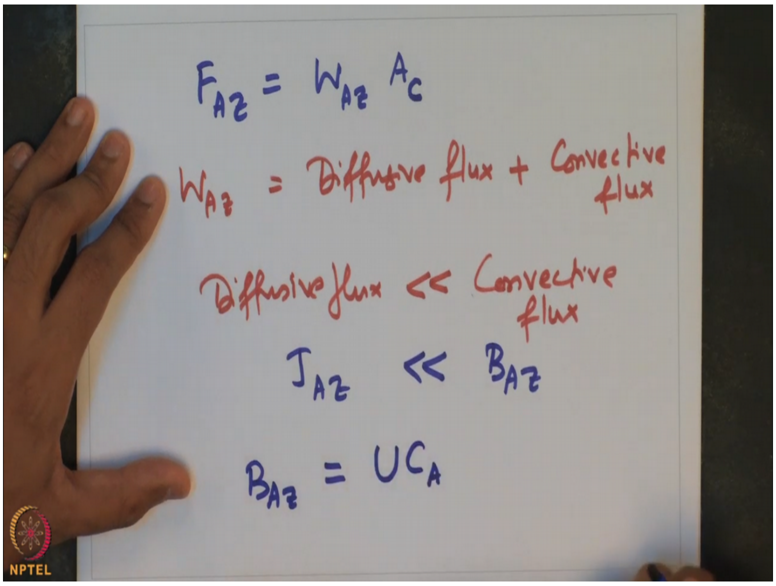

$$F_{Az} = W_{Az} A_c$$

W_{Az} = Diffusive flux + Convective flux

Diffusive flux << Convective flux

$$J_{Az} \ll B_{Az}$$

$$B_{Az} = UC_A$$

F A Z is = the flux with which the species actually is diffusing, multiplied by the cross-sectional area A c. So, this is the molar flux of the species at that location Z multiplied by the cross-sectional area. Now, how do we find what is the molar flux? The molar flux W A Z has 2 components. One is the diffusive flux, flux because of diffusion + the flux because of the bulk flow or convection because of the bulk flow.

Now, suppose if we assume that the fluid is flowing at a reasonably high rate, the superficial velocity is pretty high, then we can assume that the diffusive flux is actually much smaller than convective flux which means that the convective flux is essentially dominating the molar rate at which the species is actually flowing through the reactor at any location.

Now, if J is a is the diffusive flux, we assume that the diffusive flux is actually much smaller than the convective flux B A Z. Now, how can we express this convective flux? The convective flux B A Z is essentially given by the superficial velocity U into concentration of the species at that location.

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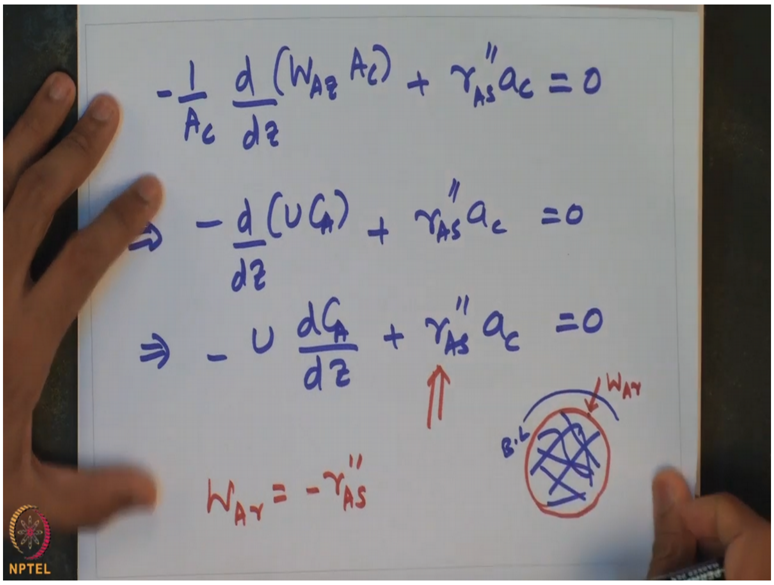

$$-\frac{1}{A_c}\frac{d(W_{Az}A_c)}{dz} + r''_{As}a_c = 0$$

$$\Rightarrow -\frac{d(UC_A)}{dz} + r''_{As}a_c = 0$$

$$\Rightarrow -U\frac{dC_A}{dz} + r''_{As}a_c = 0$$

$\Uparrow$

$W_{Ar} = -r''_{As}$

So, substituting all this into the mole balance we can find out that – 1 by A c into d by d Z of W A Z into A c + r A S double prime into A c is = 0. So therefore, from here we can find that this mole balance reduces to d by d Z of U into C A + a c = 0. Ans so, from here it will be – U d C A by d Z + r A S double prime into a c = 0. So, this is the mole balance. Now, if we know what is the rate at which the surface reaction happens as a function of concentration, then we are done.

We should be able to solve this mole balance for the packed-bed reactor design that we are considering. Now, how do we find this rate at which the reaction happens? Now, we observed in the previous lectures that if there is a catalyst particle at any location and let us say that we have a boundary layer. This is the boundary layer. And there are of course pores inside the catalyst pellet. The species which is entering through the boundary layer to the surface of the catalyst pellet, let us say that flux is given by W A r.

And at steady-state this flux with which the species is actually diffusing, species is actually being transported from the bulk to the surface of the catalyst, that W A r should essentially be = – r A S double prime. That is the rate at which the species A is actually being consumed.

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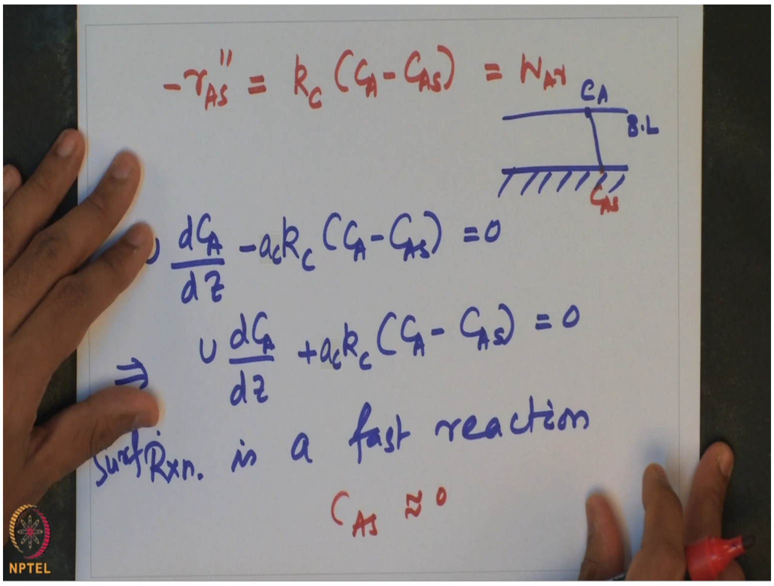

$-r_{AS}'' = k_c (C_A - C_{AS}) = W_{Ar}$

$u \frac{dC_A}{dz} - a_c k_c (C_A - C_{AS}) = 0$

$\Rightarrow u \frac{dC_A}{dz} + a_c k_c (C_A - C_{AS}) = 0$

Surf Rxn. is a fast reaction

$C_{AS} \approx 0$

So, therefore we can now say that – r A S double prime, which is the rate at which the species is being consumed is essentially = the mass transport coefficient into C A – C A S which is essentially the flux with which the species is actually being transported from bulk to the surface of the catalyst pellet. So, what we have assumed is that we have essentially now linked what we saw with the mass transport with single reaction with the packed-bed reaction now, packed-bed design now.

So, where we have said that the, if this is the surface of the catalyst pellet and this is the bulk, we essentially assume that there is a thin film boundary layer and C A is the concentration at bulk and C A S is the concentration at the surface. And we now link the process that is happening around a single pellet with the design of the packed-bed by connecting the rate at which reaction happens at any location to the flux with which the species actually is transported from bulk to the surface of the catalyst pellet.

So, if I now incorporate this into the mole balance, we will see that the mole balance essentially reduces to U d C A by d Z – k c into C A – C A S is = 0. So now, we can take out the – sign. So, this will be d C A by d Z + k c into C A – C A S is = 0. Now, we have assumed that the reaction is actually rapid, is a fast reaction, which means that surface reaction is not controlling the overall rate at which the reaction happens. What does it imply?

It means that as soon as a species reaches the surface of the catalyst pellet, the reaction would actually go to completion immediately because the surface reaction is actually very fast. Which means that the reaction is essentially happening close to the exterior periphery of the reactor. In fact, this is the reason why we actually multiplied the rate at which the reaction happens per unit area of the catalyst with external surface area per unit volume because a reaction is essentially going to happen at the exterior surface area of the exterior, close to the exterior surface of the reaction.

And therefore, if the reaction goes to completion very close to the surface then it means that the C A S can be approximately, we, can be approximated to 0. Which means, all the species which is present close to the surface would actually be consumed. Now, implementing this or incorporating this assumption reduces the mole balance to;

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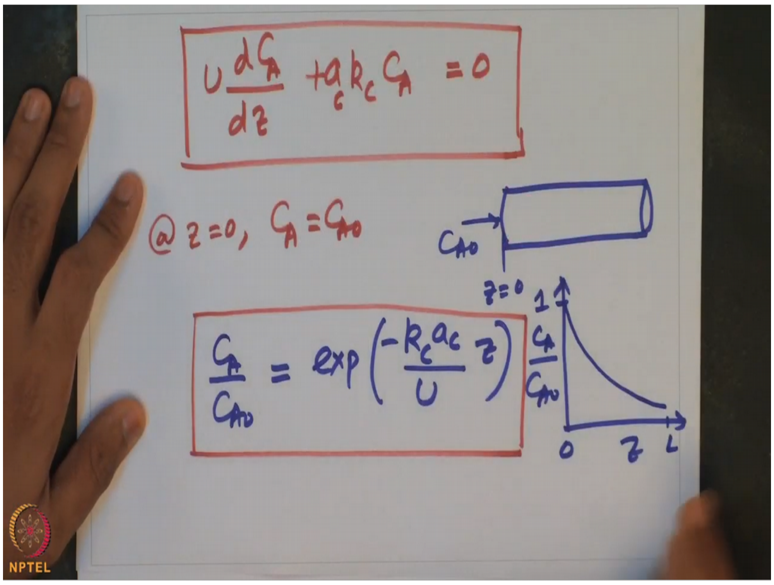

$$\boxed{U\frac{dC_A}{dz} + a_c k_c C_A = 0}$$

$@\ z=0,\ C_A = C_{A0}$

$$\boxed{\frac{C_A}{C_{A0}} = \exp\left(-\frac{k_c a_c}{U} z\right)}$$

U da C A by d Z + k c into C A is = 0. So, this is the, k c into a c into C A. So, this is the modified mole balance. And once we have this mole balance, we can now actually solve this balance. What are the boundary conditions? So, the boundary conditions are that, if this is the reactor then the concentration of the species that is actually entering the reactor, let us say at Z = 0 is essentially some C A not.

And so, the boundary conditions are essentially @ Z = 0, C A is = C A not. Now, incorporating the boundary condition and solving the model equation, we will see that C A by C A not is essentially = exponential of – k c a c divided by U into Z. So, this expression essentially captures the concentration of the species in the reactor as a function of position. Which now is a function of the mass transport coefficient, it is a function of the surface area per unit volume of the catalyst and the superficial velocity.

Now, this is valid when we have assumed that the external mass transport is actually controlling the overall rate at which the reaction happens. And the surface reaction is actually very rapid. So, let us plot this expression. So, if I now plot position versus C A by C A not. So, we will see that at Z = 0, the concentration of the species is 1. And so essentially, it exponentially falls as you go into the reactor all the way up to the exit of the reactor.

So, from here if I know what is the, what these constants are, then I can actually find out what is the concentration at different locations inside the reactor.

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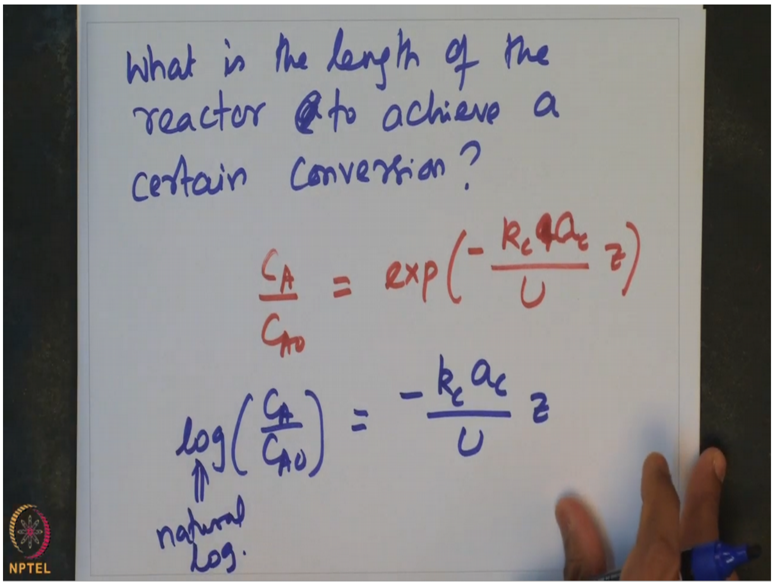

What is the length of the reactor ~~@~~ to achieve a certain conversion?

$$\frac{C_A}{C_{A0}} = \exp\left(-\frac{k_c a_c}{U} z\right)$$

$$\log\left(\frac{C_A}{C_{A0}}\right) = -\frac{k_c a_c}{U} z$$

natural log.

Now, suppose I have, I want to find out what is the length of the reactor to achieve a certain conversion. What should be the length of the reactor to achieve a certain conversion? In fact, it is an important question to ask, because, when the reaction is actually being conducted, when the reaction is actually conducted to achieve a certain productivity of a certain product species, then in that case the, what should be the length of the reactor, that is actually desired for achieving a certain conversion, is actually an important question before we attempt to design.

So, the design of a reactor, one of the important aspects of the design of the reactor is the size of the reactor itself. We want to know what is the length of the reactor that should be considered in order to achieve a certain conversion. Now, how do we find this? We can actually use the expression that is available for concentration of the species a c divided by U into Z. So, I can rewrite this expression a little bit.

I can take log on both sides. So, I can say log of, natural logarithm of C A by C not is essentially = k c a c by U into Z. This is the natural logarithm. Now, I can rewrite this expression in a slightly different fashion. Suppose I take in, I want to achieve a certain conversion? How is conversion defined?

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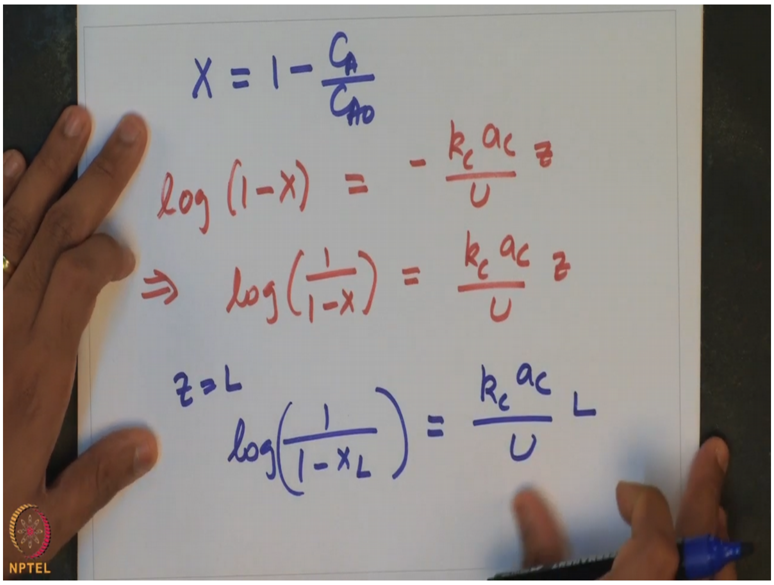

$$X = 1 - \frac{C_A}{C_{A0}}$$

$$\log(1-X) = -\frac{k_c a_c}{U} z$$

$$\Rightarrow \log\left(\frac{1}{1-X}\right) = \frac{k_c a_c}{U} z$$

$$z = L$$

$$\log\left(\frac{1}{1-X_L}\right) = \frac{k_c a_c}{U} L$$

X is the conversion and conversion is defined as 1 – C A by C A not. I can incorporate that into the model. And so, essentially it reduces to log of 1 – X is = – k c a c divided by U into Z. Or, this = log of see 1 by 1 – X is essentially = k c a c divided by U into Z. So, in order to find out what is the length of the reactor that needs to be considered to achieve a certain conversion, let us set Z = L which is the length of the reactor.

What is the conversion at that particular length? So therefore, log of 1 by 1 – X L, which is the length of the reactor, is essentially = k c a c divided by U into L. Or, the length of the reactor thus is given by;

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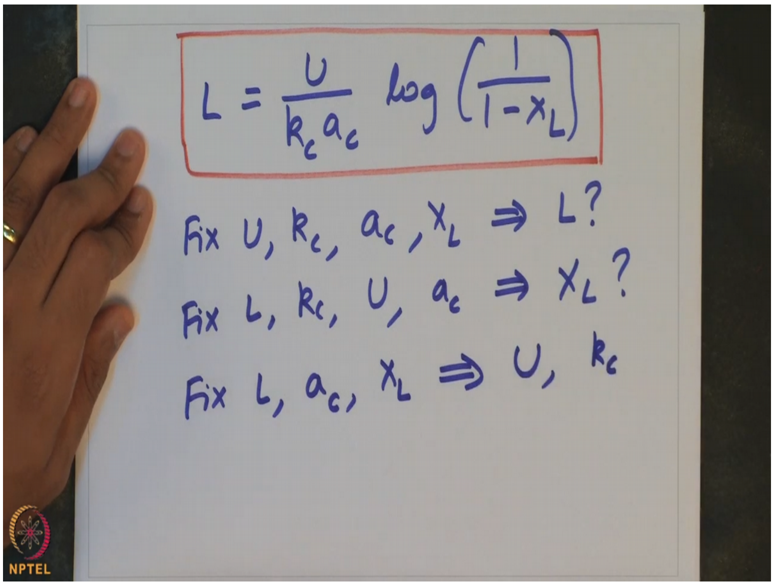

$$\boxed{L = \frac{U}{k_c a_c} \log\left(\frac{1}{1-X_L}\right)}$$

Fix $U, k_c, a_c, X_L \Rightarrow L?$

Fix $L, k_c, U, a_c \Rightarrow X_L?$

Fix $L, a_c, X_L \Rightarrow U, k_c$

U by k c into a c into log of 1 by 1 – X L. So, if I know what is the conversion that needs to be achieved and if I set the superficial velocity and the mass transport coefficient by fixing other properties, then I can actually find out what is the length of the reactor that is actually desired to achieve a certain conversion. So, I can ask a question as to, if I can fix my U, k c and a c and X L; I can ask the question what is the length of the reactor?

I can also ask another question. If I fix the length, I can fix my mass transport coefficient which is actually a function of the velocity U c and I fix my surface area per unit volume, I can ask a question as to what should be the conversion at the exit of the reactor. I can also ask another question, that if I fix my L, if I fix my area per unit volume of the catalyst and I fix my conversion, I can ask a question what should be the superficial velocity with which I have to operate, subject to the condition that this actually is a, the mass transport coefficient is a function of the superficial velocity.

I can answer any of these 3 questions. So, thus the design of the packed-bed reactor that we saw where species A is actually converted into a product steam, can actually be used to find out what is the length of the reactor which is achieved for a certain conversion. We made some crucial assumptions here where we have said that the diffusive flux is actually much smaller than the convective flux.

And this assumption can actually be relaxed while we consider the diffusive flux as well to be equally important. And we can incorporate that in the design as well. And we may solve the equations after incorporating that. And that will give us the length of the reactor for a desired conversion of diffusive flux is also equally important. The reaction that we considered in this particular model, that is the stoichiometric equation that we actually used for designing this particular packed-bed reactor design.

And so, to summarise what we have seen in this class is we looked at the packed-bed design. We made some assumptions, simplifying assumptions and we found out what is the relationship between the length of the reactor and the potential conversion that could be achieved at the product stream. In the next class we will look at how sensitive are these or what are the effects that actually would control the design of a packed-bed reactor that we have considered in this lecture. Thank you.