Chemical Reaction Engineering - II
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Module - 6
Lecture - 30
Estimation of Conversion in Packed-Bed Reactor: Example Problem

In the last lecture we started looking at an example problem from the textbook, which is essentially the hydrazine decomposition in a packed-bed reactor. So, let us continue with that problem.

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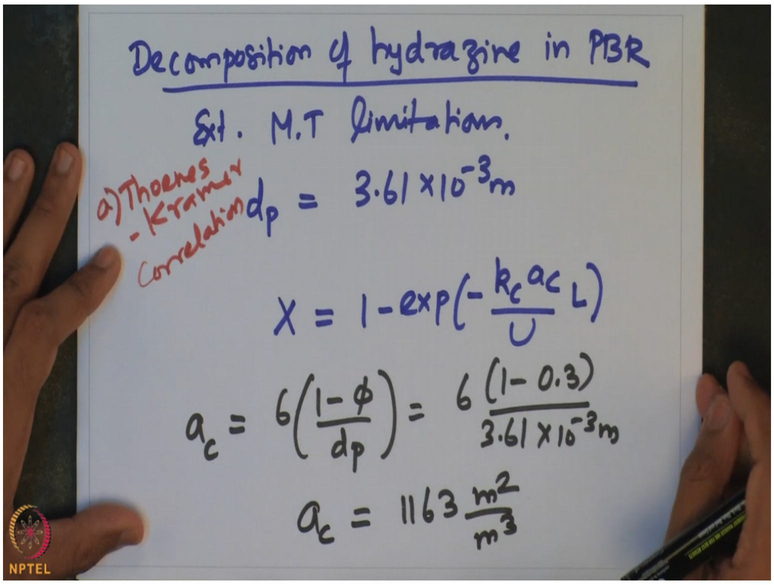

We listed down all the parameters in the last class and we said that the reactor is operated under external mass transport limited conditions. We estimated what is the equivalent particle diameter which is essentially given by 3.61 into 10 power – 3 metres. And we particularly started the Thoenes-Kramer method. We started with the Thoenes-Kramer method. We started with the Thoenes-Kramer correlation.

So, let us continue from there. So, the next step is to estimate the other parameters which are required for the conversion, for finding the conversion in the reactor. So, the conversion is given by 1 – exponential of – k c a c by U into L, where L is the length of the catalyst bed, length of the reactor bed, reactor. So, we next, let us find out what is a c which is the surface area of the reaction per unit volume.

So, a c is given by 6 into 1 – phi divided by d p, which is = 6 into 1 – 0.3 divided by 3.61 into 10 power – 3 metres. And that is essentially 1163 metre square per metre cube. So, that is the area which is actually available for the reaction per unit volume of the catalyst, unit volume of the catalyst in the packed-bed reactor.

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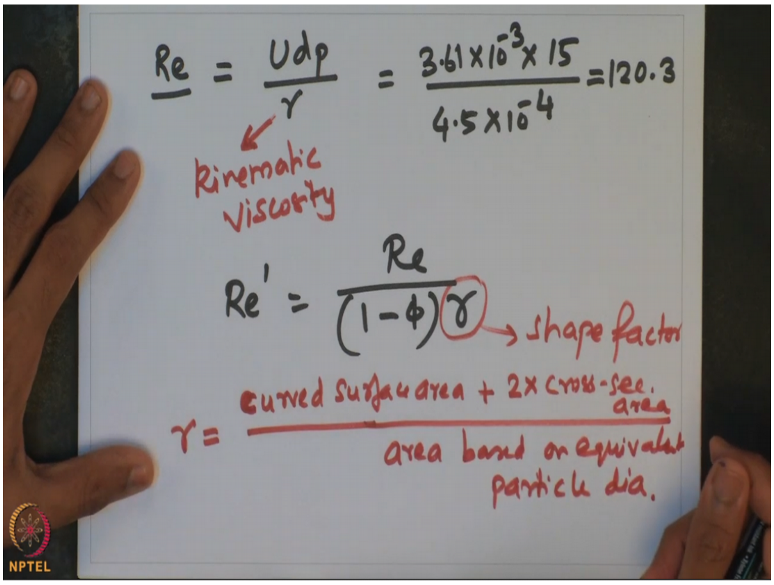

Next, let us estimate what is the Reynolds number for the packed-bed reactor system that we are looking at. So, the Reynolds number is given by U times d p divided by the kinematic viscosity. Note that this is kinematic viscosity. The kinematic viscosity is given by 4.5 into 10 power – 4 and the diameter we estimated as 3.61 into 10 power – 3 and the superficial velocity is essentially 15.

And so, from here we can find out that the Reynolds number is essentially given by 120.3. Now, that is a pretty high Reynolds number, fairly high Reynolds number. And suppose let us say we want to estimate what is the modified Reynolds number. So, R e prime is essentially given by R e divided by 1 – phi into the shape factor. Note that this is the shape factor. We now know what is the Reynolds number based on the particle diameter.

And we also know what is the porosity of the bed. Now, we need to estimate this quantity shape factor. What is the shape factor? So, the shape factor is essentially given by the curved exposed surface area or you can say curved surface area + the 2 times the cross-sectional area divided by the area based on equivalent particle diameter. So therefore, from here we can actually find out that the shape factor is essentially given by;

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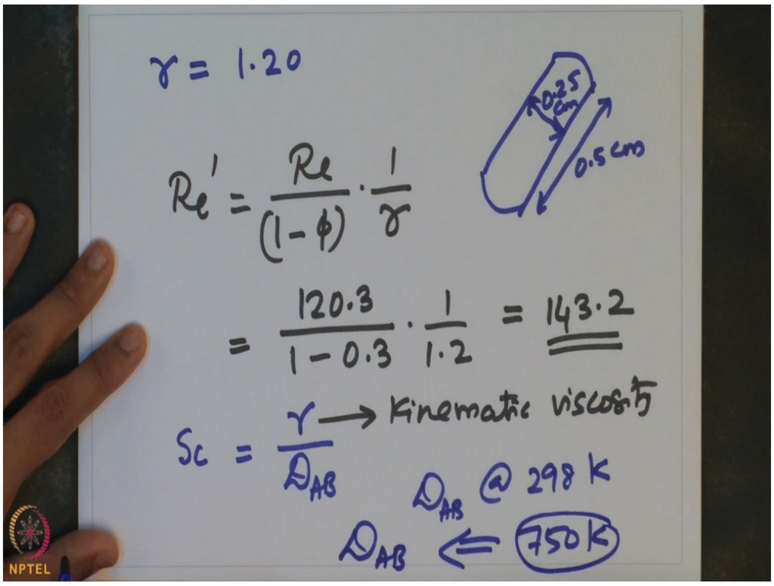

So, the shape factor is essentially given by; we can put the, we can plug-in the numbers for the diameter and the length of the bed. And we can find out that the shape factor is essentially given by 1.2. 1.2 is the shape for the cylindrical catalyst pellet that we are actually using whose diameter is essentially given by 0.25 centimetres and the length is 0.5 centimetres. So, based on the length and the diameter of the catalyst bed, we can actually find out what is the shape factor corresponding to the cylindrical catalyst pellet that we are actually using.

So, what is the next step. Once we know the shape factor, we can mediately estimate what is the modified Reynolds number R e prime, the modified Reynolds number is given by R e divided by 1 – phi into 1 by the shape factor. What is Reynolds number? Reynolds number is 120.3 divided by 1 – 0.3 is the porosity, into 1 by 1.2 and that is essentially given as 143.2. So, the modified Reynolds number which we need, which we could use in the Thoenes-Kramer correlation is essentially given by 143.2.

What is the other piece of information that we need to know? We need to know what is the Schmidt number. What is the Schmidt number? Schmidt number is essentially given by, the kinematic viscosity divided by the equimolar counter diffusivity. So, this is the kinematic viscosity. Do we have all the information? Kinematic viscosity: yes, we have, we know the numbers. What about the diffusivity?

We have diffusivity as well, but the diffusivity D A B is actually available @ 298 Kelvin. But what is the operating temperature of the reactor? The operating temperature of the reactor is actually 750 Kelvin. So, we need to find out what is the diffusivity at this temperature? What is the diffusivity of the equimolar counter diffusivity of the species at 750 Kelvin? So, let us see how to estimate that for now.

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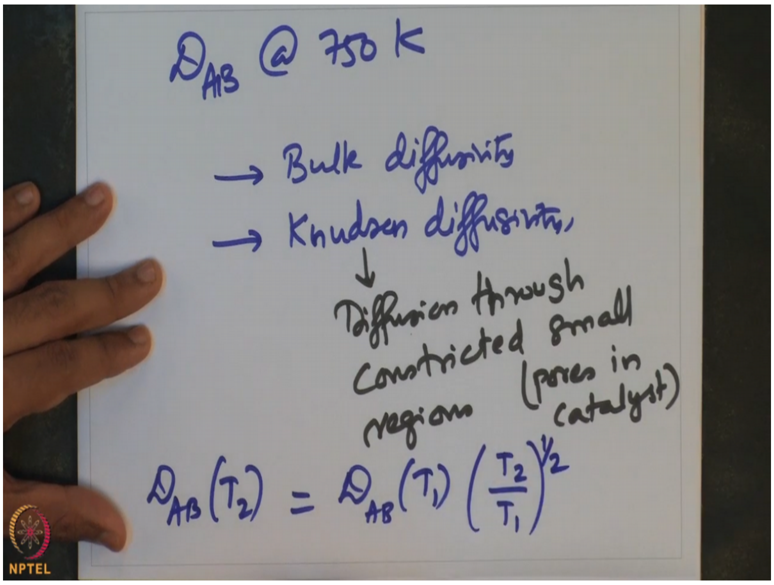

We need to find out the diffusivity @ 750 Kelvin. Now, the diffusion through the pores, the catalyst pellet actually has tiny pores which are actually present inside and the species is actually diffusing through these tiny pores. So, the diffusion of that species through these small pores is actually called as the Knudsen diffusivity. So, there are 2 diffusivities which are typically defined for gases.

One is the bulk diffusivity and the Knudsen diffusivity. So, the Knudsen diffusivity is typically for diffusion through constricted small regions. For example, like pores in a catalyst. So, now if we know the Knudsen diffusivity at a particular temperature, then we can actually find out what is the Knudsen diffusivity at a different temperature. How do we do that? We do know what is the relationship between Knudsen diffusivity and temperature.

What is that relationship? So, the Knudsen diffusivity D A B at the certain temperature T 2 is given by the Knudsen diffusivity at some other temperature T 1 multiplied by T 2 by T 1 to the power of half. So, now we know the diffusivity of the species at this temperature T1 and we can substitute in this expression and find out what is the Knudsen diffusivity at temperature T 2. So, let us do that now.

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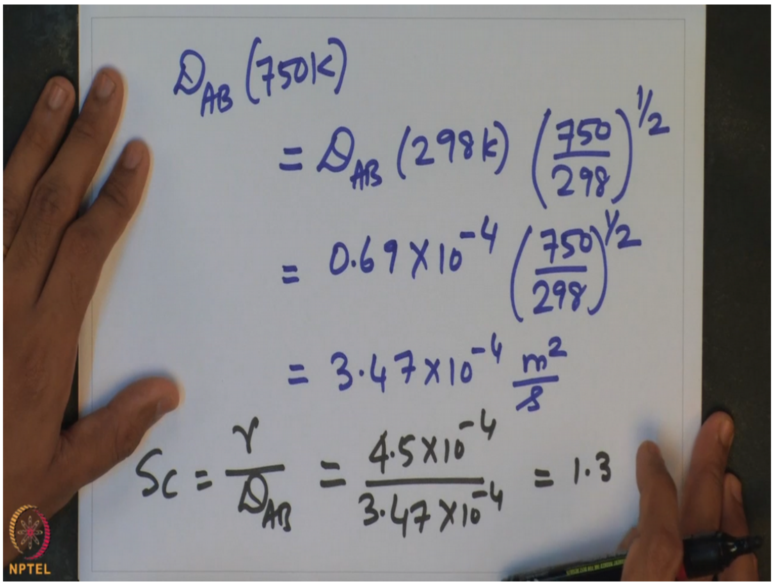

So, D A B at 750 Kelvin is essentially = D A B at 298 Kelvin multiplied by 750 divided by 298 to the power of half. And that is equal 0.69 into 10 power – 4 multiplied by 750 by 298 to the power of half. And if we calculate that, it will essentially be 3.47 into 10 power – 4 metre square per second. So, clearly you can see as the temperature is increased from 298 to 750 Kelvin.

You can see that the Knudsen diffusivity increases from 0.69 to 3.47 which is actually quite a few factor of increase in the Knudsen diffusivity of the species through the catalyst pores. So, once we know the Knudsen diffusivity, we can now estimate what is the Schmidt number, which is the kinematic viscosity divided by the Knudsen diffusivity, which is = 4.5 into 10 to the power – 4 divided by 3.47 into 10 power – 4, which is essentially = 1.3.

So, now we know what is the Reynolds number, we know what is the modified Reynolds number, we also know what is the Schmidt number. So, we can now estimate what is the modified Sherwood number, which contains the mass transport coefficient. Let us do that. So, we next use the Thoenes-Kramer correlation.

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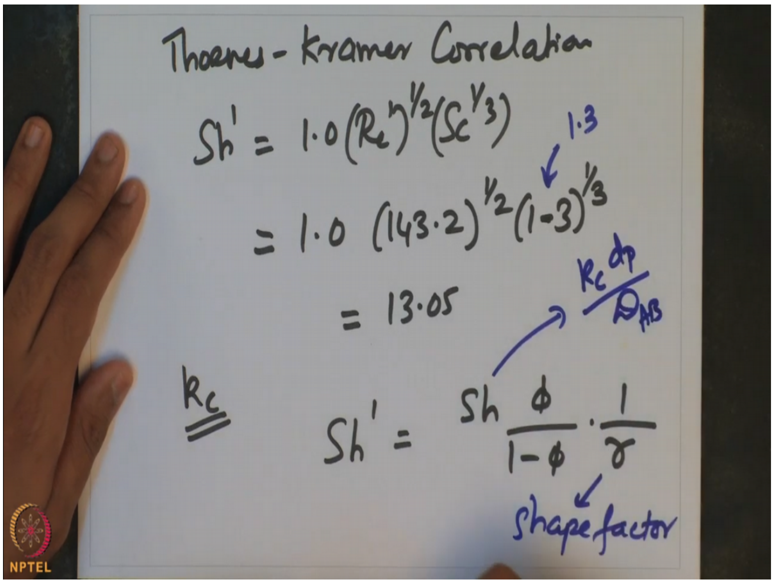

We use the Thoenes-Kramer correlation which is essentially Sherwood number, modified Sherwood number is = 1 modified Reynolds number to the power of half into Schmidt to the power of 1 by 3. We already know what is the modified Reynolds number and the Schmidt number. So, we can calculate the modified Sherwood number which is 143.2 to the power of half into 1, 1.3 to the power of 1 by 3 which is essentially 13.05. So, this is 1.3.

And so, from here we can find out what is the mass transport coefficient. How do we do that? So, modified Sherwood number is essentially given as; Sherwood number modified is given by Sherwood number into phi divided by 1 – phi into 1 by the shape factor. Note that this is the shape factor. And what is Sherwood number? Sherwood number is essentially mass transport coefficient into particle diameter, divided by the corresponding diffusivity at that temperature. So, from here we can actually find out what is the mass transport coefficient for the operating condition, at the operating conditions.

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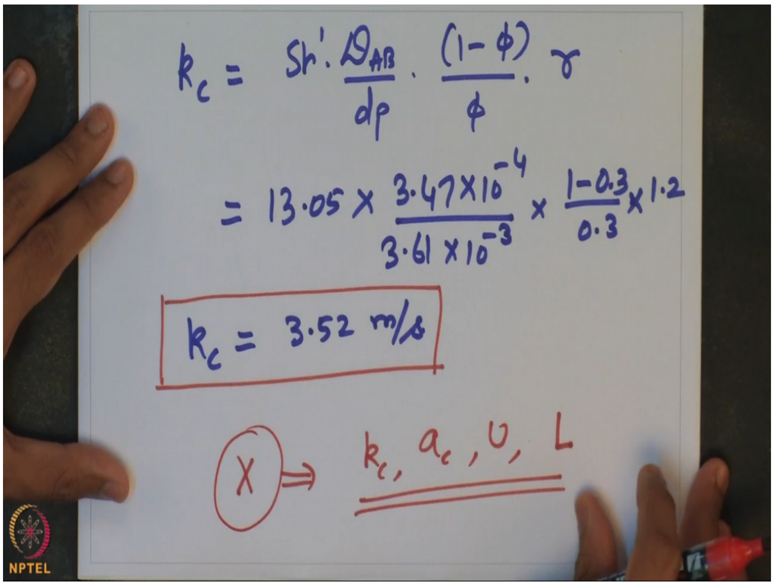

So, k c is essentially given by modified Sherwood number into D A B divided by the particle diameter into 1 – phi divided by phi into the shape factor, where phi is the porosity of the bed. Now, we estimated what is the modified Sherwood number from the Thoenes-Kramer correlation. We can substitute that here. So, that will be 13.05 into 3.47 into 10 power – 4 divided by 3.61 into 10 power – 3 multiplied by 1 – 0.3 by 0.3 multiplied by 1.2.

So, that is the shape factor. And so, that turns out to be about 3.52 metres per second. So, we know that the mass transport coefficient for the packed-bed reactor under the given operating conditions is essentially given by k c which is = 3.52 metres per second. Now, what are the quantities we need for finding out the conversion? To find the conversion we need k c, we need a c, we need the superficial velocity, we need the length of the bed.

We have all of these quantities now. We have estimated k c. We have also estimated what is the surface area per unit volume, we have, we know what is superficial velocity and we also know the length of the bed. So, now we can actually estimate what is the conversion in the packed-bed reactor under the specified operating conditions.

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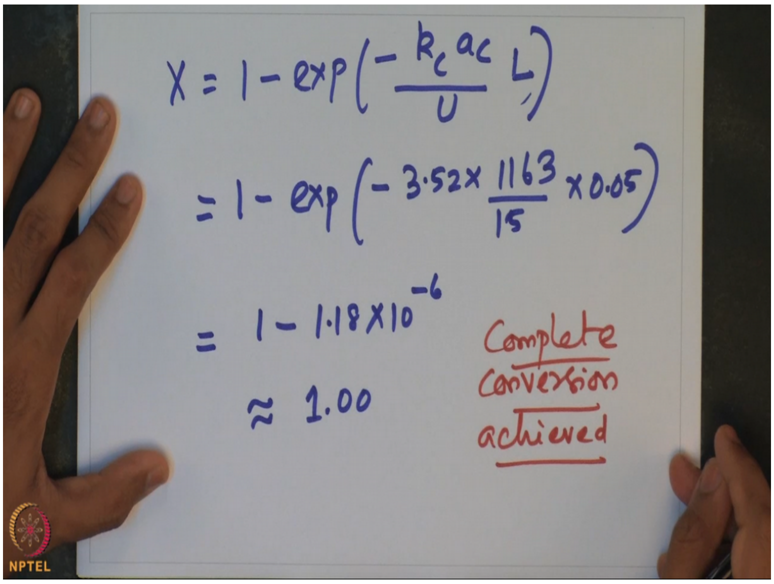

So, the conversion X is essentially given as 1 – exponential of – k c a c divided by U into L, where L is the length of the bed. And so, substituting the numbers, we will see that it is = – 3.52 into 1163 divided by 15 into 0.05 metres is the length of the bed. And so, estimating this, it will essentially be 1 – 1.18 into 10 power – 6 which is essentially approximately = 1. So, what does it suggest?

If the conversion is approximately = 1, what does it mean? It means that the species is actually nearly completely converted when it comes out in the product stream. So, the complete conversion is nearly achieved at the exit of the reactor. So, that is the estimate we get when we use the Thoenes-Kramer correlation method. Now, let us move on to the next method. We said that we can also do the same exercise by using the more generalised correlation, which is the Colburn factor method.

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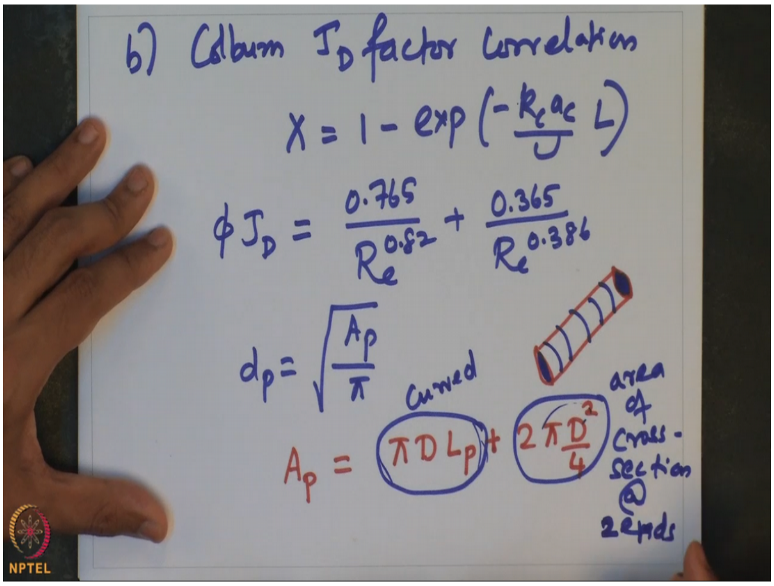

And let us estimate the conversion based on the Colburn factor method. Once again, the conversion is essentially given by U into L. And we need to estimate what is the mass transport coefficient for the condition specified based on the corresponding correlation. What is the Colburn J D factor correlation? The correlation essentially relates the Colburn J D factor to the Reynolds number at which bed is actually being operated.

And let us try to write that. So, phi into J D, phi is the porosity of the bed multiplied by J D, is essentially given by 0.765 divided by R e to the power of 0.82 + 0.365 divided by R e to the power of 0.386. Now, for using the Colburn J D factor correlation, we need to use the we need to use the specific diameter for calculating the dimensionless quantities. And the specific diameter d p is essentially given by square root of area available for the reaction divided by pi.

And so, we need to first estimate what is the external surface area which is available for the reaction divided by pi. So, once we know this, then we can go ahead and estimate the dimensionless quantities, particularly the Reynolds number. And we can find out what is the Colburn factor. And once we know what is the Schmidt number based on these properties, then we can actually find out what is the Sherwood number, from where we can actually estimate the mass transport coefficient for the system that is actually being considered.

So, let us first estimate what is the diameter of the particle which is, needs to be used for the Colburn J D correlation method. So, what is the external surface area A p? External surface area available for reaction is essentially the curved surface area which is available, + the surface area which is available, the cross section that is available at the 2 ends. So, if this is the catalyst pellet, then the area that is available for the reaction is essentially the curved surface area and the area which is available at the cross section in these 2 ends.

So, the A p is essentially sum of these 2. And this term essentially gives the curved surface area. So, this term gives the curved surface area, and this term gives the area available at the cross section at 2 ends. So, this pi D square by 4 is the area of this cross section and that because there are 2 ends we multiply it by 2. So, that gives the area, surface area available external surface area available for the reaction. So, based on this we can calculate what this d p diameter is.

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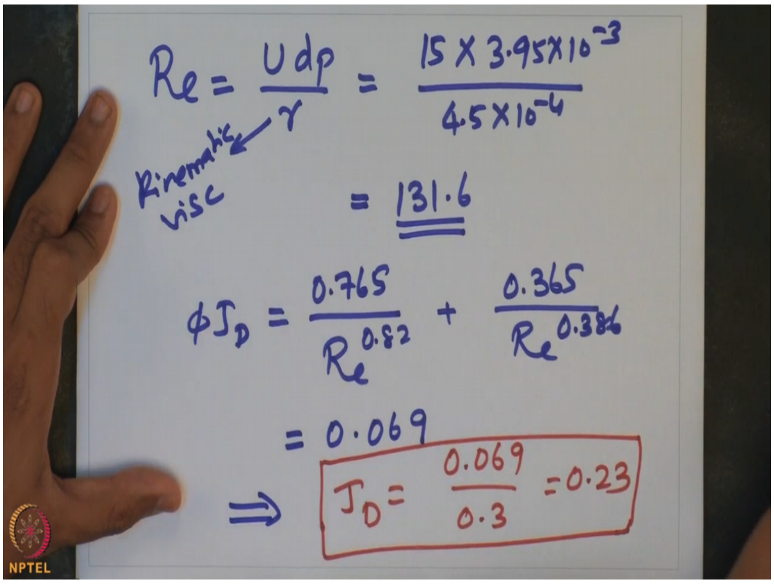

So, d p is essentially given by square root of pi D L p + pi D square by 2 divided by pi, which is = square root of D L p + D square by 2. So, plugging in the numbers, that will be, 0.25 into 10 power – 2 multiplied by 0.5 into 10 power – 2, + 0.25 into 10 power – 2 divided by 2. And that is given by 3.95 into 10 power – 3 metres. So, that is the diameter of the particle which we need to use for estimating the dimensionless quantities for the J D correlation factor, J D factor correlation.

So, what is the next step? We need to find out what is a c, which is the area available per unit volume. That will be 6 into 1 – phi divided by the d p, which is = 6 into 1 – 0.3 divided by 3.95 into 10 power – 3 which is essentially 1063 metre square per metre cube. So, that is the surface area per unit volume which is actually available for the reaction. The next step is to estimate the Reynolds number.

So, the Reynolds number is given by U d p divided by nu. Note that this is kinematic viscosity. Which is essentially 15 into 3.95 into 10 power – 3 divided by 4.5 into 10 power – 4 which is essentially = 131.6. That is the Reynolds number. And from using the correlation phi J D = 0.765 divided by Reynolds number to the power of 0.82 + 0.365 divided by Reynolds number to the power of 0.386.

Substituting the values of the Reynolds number we will find that 5 times J D, which is the porosity times the Colburn factor is essentially = 0.069. So, from here we can find out that the J D which is the Colburn factor is essentially given by 0.069 divided by 0.3, which is = 0.23. So, once we know J D the Colburn factor, we can find out what is the Sherwood number. Because the Colburn factor, Sherwood number, Schmidt number and the Reynolds number are actually related. So, let us look at what the relationship is.

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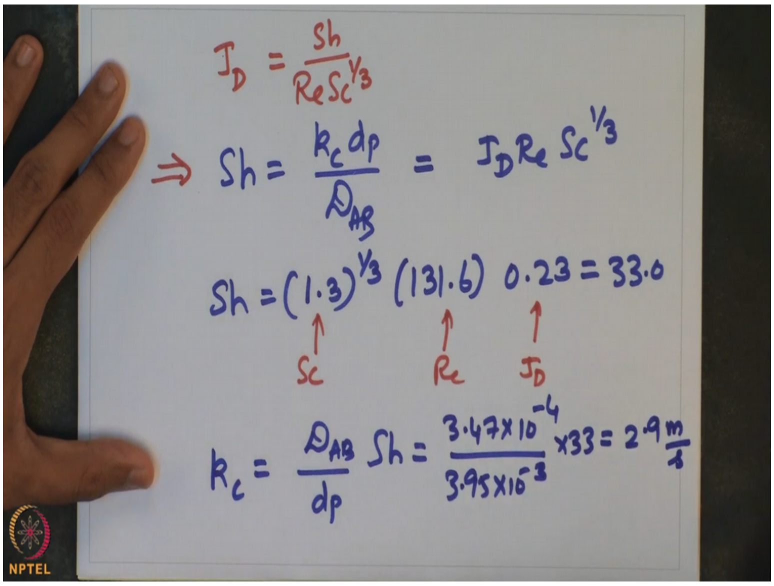

So, the Colburn Factor J D is essentially given by Sherwood number divided by Reynolds number into Schmidt to the power of 1 by 3. So, from here, we can find out that the Sherwood number is = k c d p by D A B is essentially = J D into R e into Schmidt number to the power of 1 by 3. Now, the Schmidt number that we calculate in the Thoenes-Kramer correlation case will be same as what it is in this case is well.

Because the Schmidt number is just a ratio of the kinematic viscosity to the Knudsen diffusivity at that temperature. And that is independent of the particle diameter. So therefore, the Schmidt number that we calculated earlier can be directly used to find out the Sherwood number using the Colburn J D factor correlation. Let us do that. So, from here, Sherwood number is essentially = 1.3 to the power of 1 by 3, Schmidt number to the power of 1 by 3 into 131.6 which is the Reynolds number and 0.23 is the J D factor.

So, this is the Schmidt number, J D Colburn factor. And so, from here we find out that Sherwood number is essentially = 33. So, from this we can find out the mass transport coefficient, which is D A B by d p into Sherwood number, which is = 3.47 into 10 power – 4 divided by 3.95 into 10 power – 3 multiplied by 33 which is = 2.9 metres per second. So, that is the mass transport coefficient if we use the Colburn J D factor correlation for finding the Sherwood number and thereby finding the mass transport coefficient.

So, once we know the mass transport coefficient, we can actually find out the conversion, where the conversion is essentially related to the mass transport coefficient, area per unit volume and the superficial velocity and length of the catalyst belt. So, let us see how to estimate that. So, the mass transport coefficient k c, we already know.

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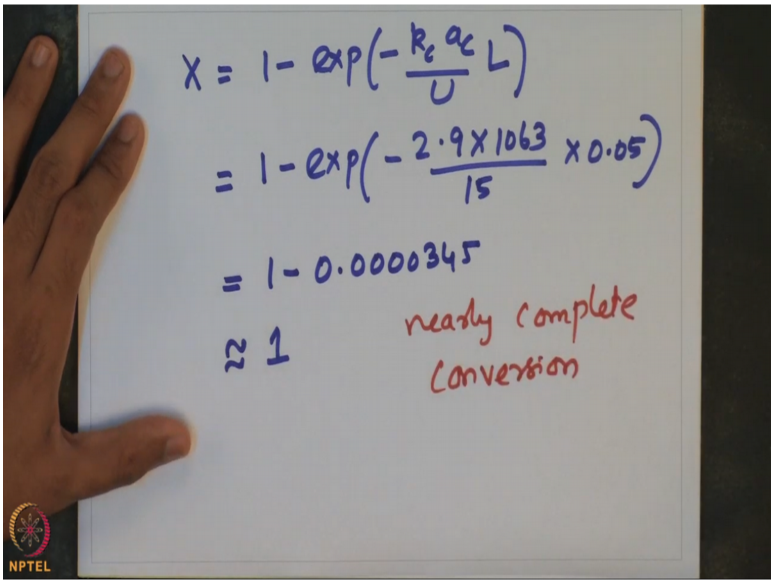

So, the conversion X is essentially going to be, 1 – exponential, – k c a c divided by U into L, which is the length of the bed. And that is essentially given by 1 – exponential of – 2.9 into 1063 divided by 15 into 0.05. And from here we can find out that the conversion is essentially given by 0.0000345, which essentially is approximately = 1. So clearly, this method also predicts that it is actually nearly complete conversion.

So, what the calculation suggests is that the length of the bed that is used for the decomposition of hydrogen, the design that is used in the packed-bed, whatever length that is considered for this particular bed which is 0.05 metre is actually sufficient to achieve nearly a complete conversion of the feed stream. So, this is a, this shows an interesting example of how mass transport coefficient and design actually plays an important role and how we can actually find out what is the conversion for the given bed under the operating conditions that is specified.

So, what we have seen in the external mass transport limitations conditions where we looked at how external mass transport resistances can be quantified. And to summarise that aspect, particularly we looked at;

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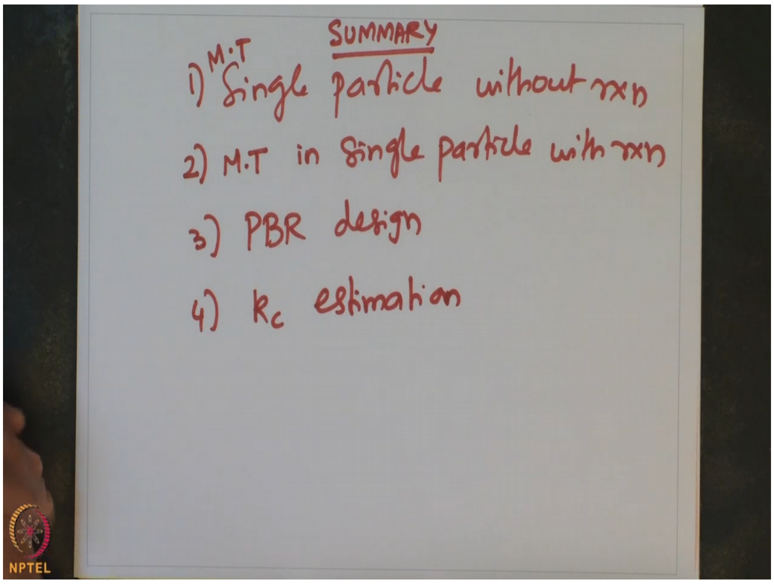

So, we specifically looked at the single particle case, single particle without reaction. We looked at mass transport to single particle without reaction. So, this is essentially the summary of the external mass transport limitations it will consider. And then the second aspect we considered is essentially mass transport in single particle with reaction. And the third case we considered is essentially the packed-bed reactor design.

And then we actually looked at how to estimate the mass transport coefficient, mass transport coefficient estimation. So, these are the 4 specific aspects we have looked at under the external mass transport limited condition, operation of the reactors under external mass transport limitations and how to characterise this. In the next class, we will start looking at the overall effectiveness factor which essentially captures the effects of the external mass transport diffusion and the internal mass transport diffusion along, simultaneously along with the effects of the surface reaction.

The effectiveness, overall effectiveness factor can actually be used to identify when the reaction or the overall rate is controlled by the external mass transport limitations or the internal mass transport limitations or the surface reaction. So, that is what we will see from the next lecture. Thank you.