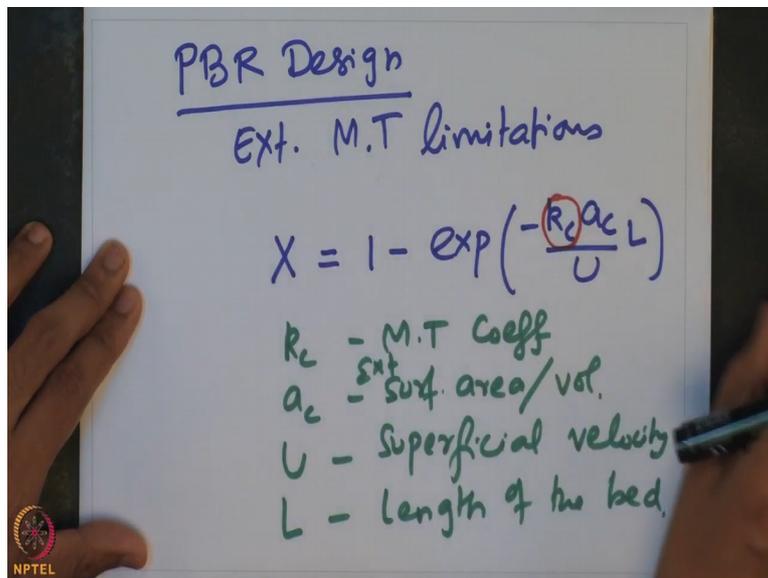


Chemical Reaction Engineering - II
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Module - 6
Lecture - 29
Mass Transfer Coefficient in Packed-Beds

In the last lecture we looked at the design of packed-bed reactor which is operated under external mass transport limitations. We particularly looked at what is the way to achieve the or find the expression for the conversion as a function of the mass transport coefficient.

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And we found that conversion is essentially given by $1 - \exp\left(-\frac{k_c a_c L}{U}\right)$. So, k_c is the mass transport coefficient, mass transport coefficient for the species to diffuse from bulk to the surface of the catalyst pellet. And a_c is essentially the surface area per unit volume, external surface area per unit volume. And U is the superficial velocity, L being the length of the bed.

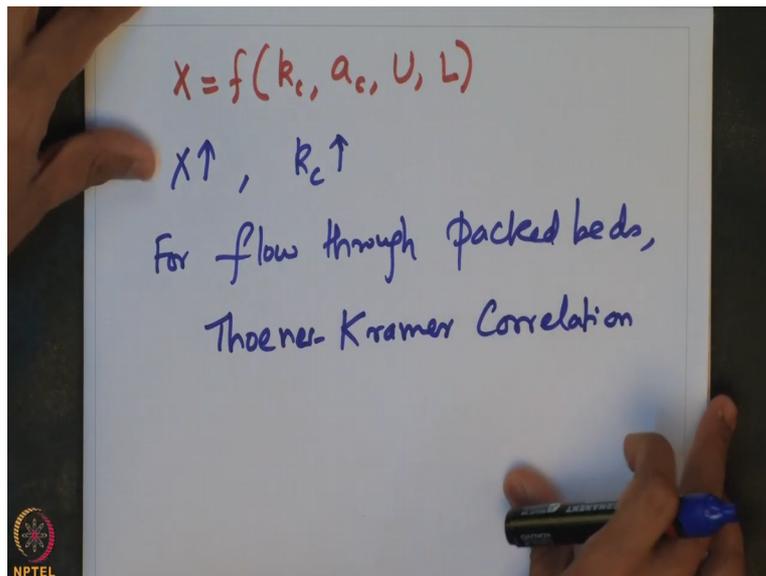
So, often the question is how do we improve the conversion of a given reactor. So, we know what is the conversion as a function of the mass transport coefficient, external surface area which may be available in the bed and the superficial velocity. So, in, if we have to find out how to improve the conversion for a given reactor and given catalyst and given reaction, whose intrinsic kinetics is fixed and the reactor is operated under external mass transport limitations.

So, 1 way to do that is actually by tweaking this mass transport coefficient. If we can improve the mass transport coefficient somehow, if we can improve the mass transport coefficient, then we will be able to improve the conversion to a great extent. So, let us see how to do that. So, we first have to find out how the mass transport coefficient depends on the other operating parameters.

Now earlier, in couple of lectures ago, we looked at how mass transport coefficient depends upon the operating conditions when the fluid is actually flowing past a single particle or single catalyst pellet. Now, the fluid is actually flowing past through a packed-bed reactor. So, therefore we need to look at how mass transport coefficient is affected in the whole reactor system which is actually packed with catalyst, unlike the case where we looked at before where it was just a single catalyst pellet.

In that, when the, in the case of single catalyst pellet, we actually took advantage of the boundary layer analogy. And we related the mass transport coefficient which is present in Sherwood number to the Reynolds number and Schmidt number using the Frossling correlation. But, that correlation unfortunately cannot be used here because this the this system is flowed through the packed-bed where there are several particles which are actually packed inside the bed. So, let us look at how to characterise mass transport coefficient or how to estimate mass transport coefficient in a packed-bed reactor design.

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So clearly, the conversion is a function of the mass transport coefficient, area per unit volume available for reaction, superficial velocity and the length of the bed. Now, suppose if I want

to improve the conversion, 1 way I could do is I can actually improve the mass transport coefficient. Now, how do we estimate mass transport coefficient? There are specific correlations which are actually available for flow through bends, for flow through packed-beds.

The correlation which actually captures the mass transport coefficient is what is called as the famous Thoenes-Kramer correlation. In fact, this correlation is valid for fluidized bed reactors as well. And the correlation is Sherwood number;

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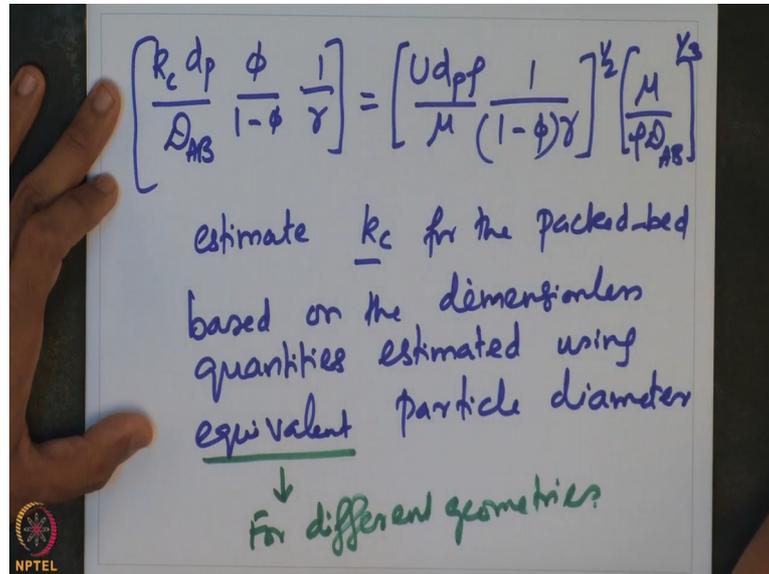
The image shows a whiteboard with handwritten equations in blue ink. At the top, the modified Sherwood number is given as $Sh' = 1.0 (Re')^{1/2} (Sc')^{1/3}$, with a circled 'Sh' and 'T-K Cor.' written to the right. Below this, the equation $Sh' = Sh \frac{\phi}{1-\phi} \frac{1}{\gamma}$ is written, with arrows pointing from ϕ to 'porosity' and from $\frac{1}{\gamma}$ to 'Shape factor'. The modified Reynolds number is defined as $Re' = \frac{Re}{(1-\phi)\gamma}$, and the modified Schmidt number is $Sc' = \frac{\gamma}{D_{AB}}$. An NPTEL logo is visible in the bottom left corner of the whiteboard image.

Some modified Sherwood number is = some modified Reynolds number into Schmidt number to the power of 1 by 3. So, this modification is essentially to account for the fact that the system that we are considering is a full packed-bed which contains several particles. So, this is essentially the Thoenes-Kramer correlation. And let is define what these parameters are. So, the Sherwood number, modified Sherwood number is the Sherwood number of the system, multiplied by phi which is the porosity, divided by 1 – phi into 1 by what is called as the shape factor.

So, phi is the porosity of the bed and this is the shape factor. We will see in a bit, we will see an example where how to actually estimate the shape factor. And the next parameter here is the modified Reynolds number which is essentially given by R e divided by 1 – phi into the shape factor. Once again, phi is the porosity of the bed and this quantity is the shape factor. And Schmidt number essentially is the same as what we saw before, which is the kinematic viscosity divided by the corresponding diffusivity at the operating conditions.

So now, if we know the parameters of a given system, then we should in principle be able to estimate the modified Sherwood number, modified Reynolds number and modified Schmidt number. So, if I now, plug these in, into the Thoenes-Kramer correlation, plug the modified expressions for these different dimensionless quantities;

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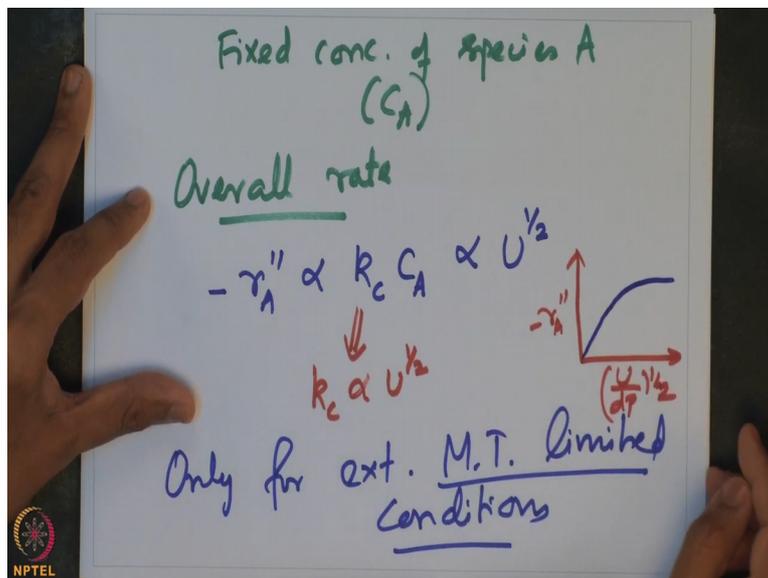
We will see that the Thoenes-Kramer essentially boils down to k_c into equivalent particle diameter d_p multiplied by ϕ divided by $1 - \phi$ into 1 by shape factor. And that should be $= U d_p \rho / \mu$, which is nothing but the Reynolds number based on the particle diameter, to the power of half into $\mu / \rho D_{AB}$ which is this Schmidt number to the power of $1/3$.

So, now if we know the parameters as a function of the particle diameters, if we estimate the parameters as part of the as taking the particle diameter as a representative diameter, then we should be able to express the correlation in terms of the particle diameter and taking into account the bed property such as porosity and the shape factor which takes into account different geometries.

So, thus we can actually estimate, this correlation can be used to estimate the mass transport coefficient for the packed-bed based on the dimensionless quantities estimated using the equivalent particle diameter. And we can account the presence of the bed using the corresponding porosity and the other properties. So, equivalent particle diameter essentially helps in using this correlation for different geometries.

Suppose, if I keep all the properties constant, if I keep all the properties constant for the whole system that is a catalyst bed, flow rate, so on and so forth, temperature, etcetera. Then, as we estimated for the single particle case, even here as well, the mass transport coefficient k is actually proportional to U to the power of half. That is the superficial velocity to the power of half.

So therefore, by actually changing the superficial velocity, one can actually achieve a higher mass transport coefficient by increasing the superficial velocity. Of course, one cannot increase it significantly, it depends upon the nature of the setup that is being used. So, there is always an upper, there may be an upper limit on how much the superficial velocity can actually be increased. So, suppose I fix the concentration, suppose for a fixed concentration;
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Concentration of let us say species A which is undergoing reaction, let us say that fixed concentration in some C_A , then the overall rate is now going to be proportional to the mass transport coefficient into the concentration of the species. And we know that from the correlation from the Thoenes-Kramer correlation, we know that k_c is actually of proportional to the superficial velocity to the power of half.

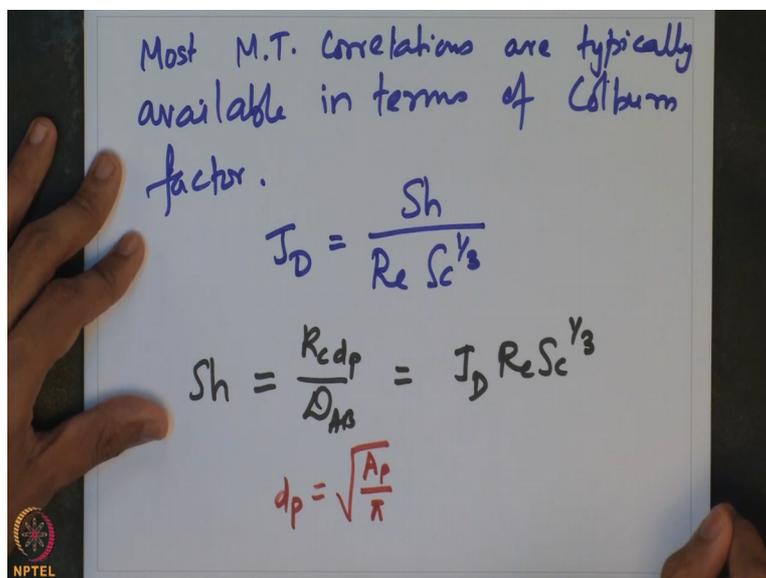
And therefore, the overall reaction rate is essentially going to be proportional to the square root of the superficial velocity. So, by controlling the superficial velocity with which the species is actually, feed stream is flowing through the reactor, one should be able to actually modulate the observed reaction rate for the reaction that is happening in the packed-bed, packed with the catalyst.

Now, note that this is work, this works only if this a, it is a mass transport limited conditions. This is valid only for external mass transport limited conditions. Now, if we, suppose let us say we increase the velocity significantly, then it may turn out that the external mass transport limitations are no more there. So, therefore the dependency of the overall reaction rate on the velocity with which the fluid is actually flowing is valid only when the external mass transport limited regime.

And in fact, we looked at for a single particle case, we looked at the situation where, if I look at U by d_p power of half and the overall rate which we observe that there is a region where it is external mass transport limited control after which the overall rate at which the reaction happens is independent of the velocity. So clearly, there is a, an upper limit to which the velocity, superficial velocity can be increased, where the reaction rate is a function of the superficial velocity.

After that point, how much ever the superficial velocity is increased, the overall rate increase is going to be very marginal because the external mass transport limitation assumptions is no more valid.

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Most M.T. Correlations are typically available in terms of Colburn factor.

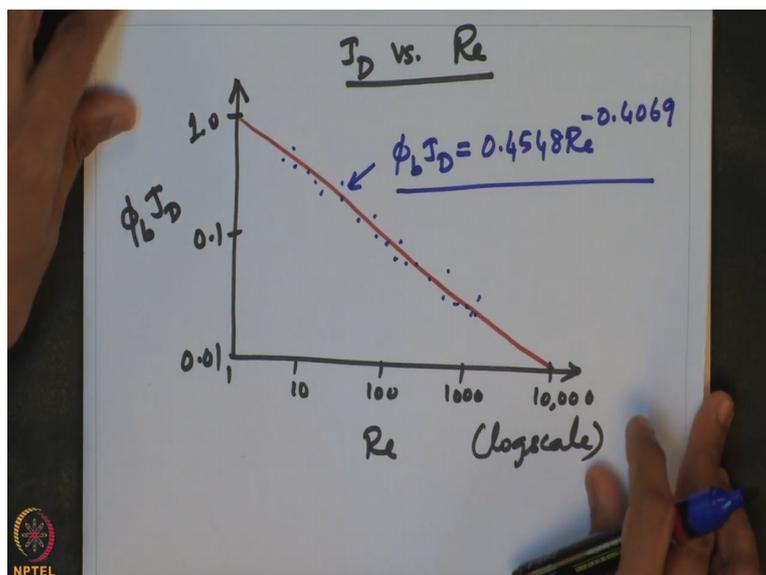
$$J_D = \frac{Sh}{Re Sc^{1/3}}$$
$$Sh = \frac{k_c d_p}{D_{AB}} = J_D Re Sc^{1/3}$$
$$d_p = \sqrt{\frac{A_p}{\pi}}$$

So, for most of the, most mass transport correlations are typically available in terms of a factor called Colburn factor. And the symbol that is used for Colburn factor is J_D , which is essentially given by Sherwood number divided by Reynolds number into Schmidt number to the power of 1 by 3. So, instead of Thoenes-Kramer another way to estimate the mass transport coefficient k_c is by estimating the Colburn factor.

So, if we know the Colburn factor, then we can actually use this expression here. You can use this expression to find out the Sherwood number which is essentially given by k_c divided by D_{AB} into the particle diameter. And that is essentially J_D into Re into Schmidt number to the power of $1/3$. Note that for this kind of a correlation where J_D is used the particle diameter is typically given as the available area for the reaction divided by π .

It is not the equivalent particle diameter that is used. The one that usually works is the particle diameter based on the available area for the reaction to happen. Let us say the external surface area where the reaction happens when there is external mass transport limitations. So, this Colburn factor of course is a function of the Reynolds number and we will, let us see how that depends on the Reynolds number which actually captures the velocity with which the fluid stream is actually flowing through the reactor.

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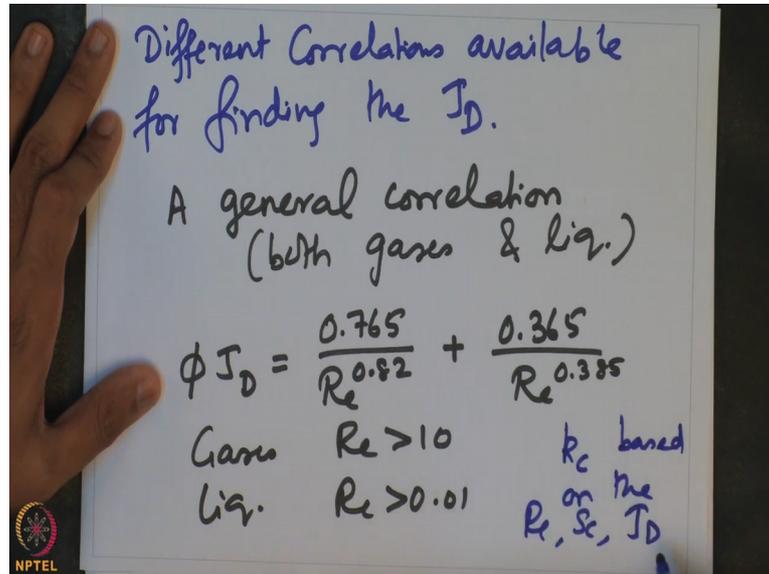


So, if I now use a log scale for Reynolds number, let us say 1 and 10 and so on, up to let us say 10,000 here. And this is log scale. And if I now plot $\phi_b J_D$, which is the porosity of the bed, then it actually follows an inverse power law behaviour. So, the typical curve or the correlation between the $\phi_b J_D$ and Reynolds number is essentially an invert.

And most of the experimental data that has been done for finding the Colburn factor as the function of Reynolds number, they will essentially fall along this inverse power law behaviour. And in fact, the, this can actually be found, the relationship of this line is essentially given by $\phi_b J_D = 0.4548$ into the Reynolds number to the power of -0.4069 . So, this is the correlation.

Now, there are many different types of correlations which are actually available for the flow through packed-bed for estimating the Colburn factor for flow through packed-beds under different conditions. And there are, there is a correlation which essentially summarises all these different correlations which are available for different conditions and different systems.

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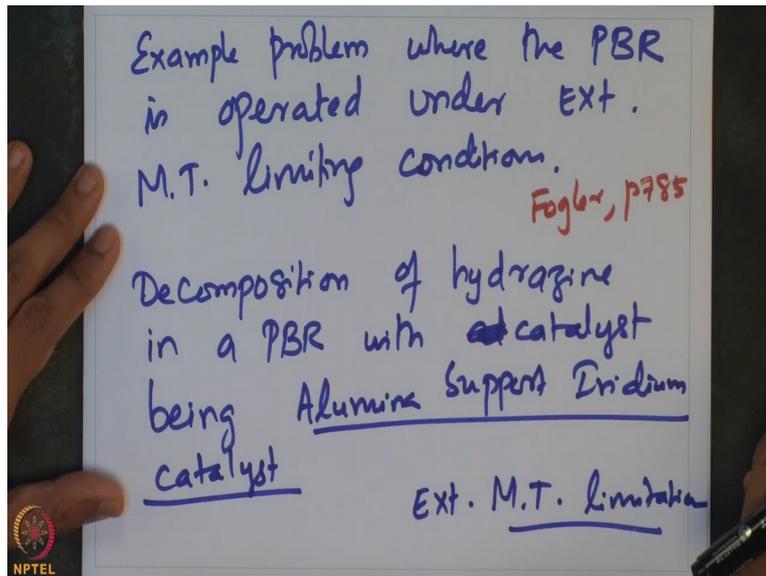


So, different correlations available for finding the Colburn factor. So, there is a generalised correlation which is applicable for both gases and liquids under different range of Reynolds number. So, a general correlation which is applicable for both gases and liquids is essentially given by 5 times J_D , which is again the porosity of the bed, is = 0.765 divided by Reynolds number to the power of 0.82 + 0.365 divided by Reynolds number to the power of 0.385.

And this is typically valid for gases when the Reynolds number is greater than 10. And for liquids, when the Reynolds number is actually greater than 0.01. And normally when the reactor is operated, the Reynolds number is typically for gas streams is typically more than 10 and for liquid is typically more than 0.01. So, therefore the general correlation that is here is actually valid for, wide range of Reynolds number for both gases and liquids.

And therefore, this correlation is actually quite widely used to estimate the mass transport coefficient based on the Reynolds number, Schmidt number and the Colburn factor J_D . So, once we know the Colburn factor which actually uses the Reynolds number and Schmidt number to relate the Sherwood number to Colburn factor. We can actually find out what is the mass transport coefficient for a given condition. So, let us next look at a very specific example.

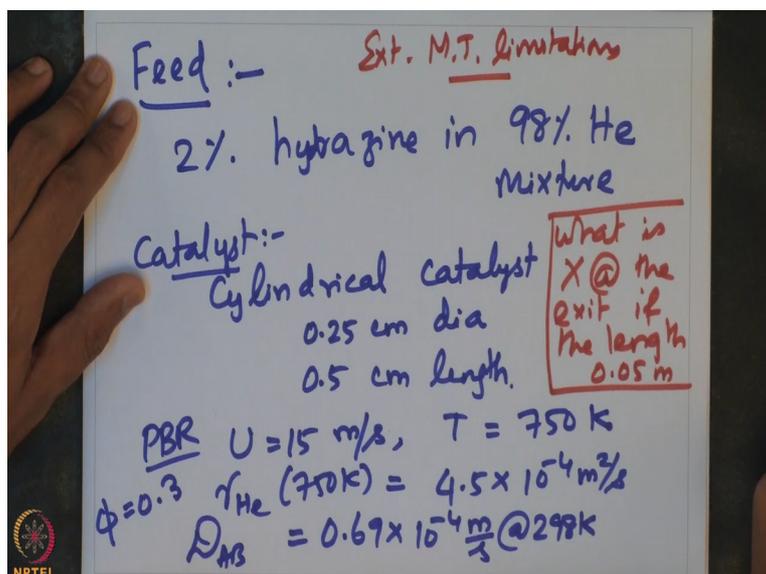
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We will take an example problem where the packed-bed reactor is operated under external mass transport limited conditions. So, the specific example we are going to look at essentially is been taken from the textbook, in Fogler textbook page number 785. And we are going to specifically look at the case of decomposition of hydrogen in a packed-bed reactor with catalyst being Alumina support Iridium catalyst.

So, that is the catalyst that is used. And we assume that the reaction is conducted under external mass transport limitations. Assume that it is conducted under external mass transport limitations. And let us look at what are all the parameters that are actually available, what are the properties of the system that are actually available.

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So, the feed is essentially 2% hydrazine in 98% helium mixture. That is the feed. And the catalyst properties are: it is a cylindrical catalyst and the diameter of the catalyst is 0.25 centimetre dia and the length of the catalyst is 0.5 centimetre. And it is, and the properties with which the reactor is operated is, the superficial velocity is 15 metres per second. And the temperature at which the reactor is operated is 750 Kelvin.

And we assume that the kinematic viscosity of helium with at 750 Kelvin, is essentially given by 4.5×10^{-4} metre square per second. And we also assume that the equimolar counter diffusivity of the species is 0.69×10^{-4} metres per second at 298 Kelvin. And we assume that the porosity of the bed is actually 0.3. So, the question that we need to answer, the question is, what will be the conversion?

What is the conversion at the exit if the length of the bed is = 0.5, if the length is essentially 0.05 metres is the length of the reactor. So, we need to find out what is the conversion. So, how do we go about solving this problem? We have all the parameters. And we have said that it is actually external mass transport limitations. So, how do we solve this problem? So, when we looked at the packed-bed reactor design, we actually found out what is the relationship between the conversion and the mass transport coefficient.

So, let us start looking at that. So, in a packed-bed reactor under external mass transport limitations we found that the conversion essentially is given by;

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

$k_c?$, $a_c?$

1) Thoenen-Kramer Correlation
 2) Colburn J_D factor Correlation

From 1) $Sh', Re', Sc \rightarrow k_c$
 From 2) $Sh (dp), Re \Rightarrow J_D, Sc \Rightarrow k_c$

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$1 - \exp(-k_c a_c L / U)$ where L is the length of the reactor. So, we need to find out what is k_c . We need to find out the area per unit volume and superficial velocity is given. So, once we find these 2, we are done. We should be able to estimate what is the conversion of the reactor at the exit of the packed-bed reactor, whose length is essentially L . So, L is given, U is given, we need to find k_c and a_c .

So, how do we find k_c . We can use 2 methods to do that. We describe 2 different methods by which we can estimate k_c . Where first approach for estimating k_c is by using the Thoenes-Kramer correlation. But, we can also use the other method of the Colburn J_D factor correlation. You can use correlation for finding the Thoenes-Kramer and Colburn J_D factor.

So, what we will do is, we will basically use both these approaches and we will find out what is the mass transport coefficient under the given conditions when we use Thoenes-Kramer correlation and also when we use the Colburn J_D factor correlation. And we will compare what is the conversion that we will achieve by using these 2 different approaches or different correlations for finding the mass transport coefficient.

Now, what are the dimensionless quantities we need to estimate? Suppose if it is the Thoenes-Kramer correlation approach, then what are the quantities we need? We need the modified Sherwood number which contains the mass transport coefficient. In order to find the modified Sherwood number, we need to find out the modified Reynolds number. We need to find out what is the Schmidt number.

But, suppose if J_D is the Colburn J_D factor, then we need to find out what is the Sherwood number based on the corresponding definition of d_p particle diameter. And we need to find out what is the Reynolds number to find the, which give, which essentially is used to find the Colburn factor J_D . And then we need Sherwood number to calculate the mass transport coefficient based on these 4 quantities.

That is, by Reynolds number, J_D , Smith number and Sherwood number which essentially contains the mass transport coefficient. So, if we know these 3, then we can actually find out what is the mass transport coefficient. And once again, in this case as well, once we know the modified Sherwood number from the correlation we can find out what is the mass transport coefficient. So, let us start by the first approach of using the Thoenes-Kramer correlation.

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1) Thoenes-Kramer Correlation Approach.

$$Sh' = 1.0 (Re')^{1/2} (Sc)^{1/3}$$
$$Re' = \frac{Re}{(1-\phi)\gamma} = \frac{U d_p}{\nu} \frac{1}{(1-\phi)\gamma}$$

kinematic visc. shape factor

(Cylindrical \Rightarrow) Equivalent diameter

So, what is the Thoenes-Kramer correlation? The Thoenes-Kramer correlation is essentially given by the modified Sherwood number is = 1 into modified Reynolds number to the power of half into Schmidt number to the power of 1 by 3. Now, what is the Reynolds number? Reynolds number, modified Reynolds number is essentially given by Reynolds number by, Reynolds number based on particle diameter divided by 1 – phi into the shape factor.

And that is = U into the equivalent particle diameter d p divided by the kinematic viscosity nu, that into 1 by 1 – phi into the shape factor. Now, note that this is kinematic viscosity and this is the shape factor. So, what is the first step in doing this? We need to estimate what is the equivalent particle diameter. Because the particle that we have is actually a cylindrical particle. And this definition is essentially for spherical particle.

So, we need to find out what is the equivalent diameter of the particle that is actually being used. Now, how do we find the equivalent particle diameter. We can actually do what is called as the volume averaged. So, the equivalent particle diameter d p;

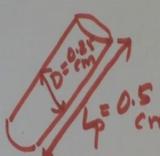
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Equivalent particle diameter
(d_p) using volume averaging.

$$d_p = \left(\frac{6V}{\pi} \right)^{1/3}$$

$$= \left(\frac{6 \pi \frac{D^2}{4} \cdot L_p}{\pi} \right)^{1/3}$$

$$= \left[\frac{6}{4} (0.25 \times 10^{-2})^2 (0.5 \times 10^{-2}) \right]^{1/3}$$

$$= 3.61 \times 10^{-3} \text{ m}$$


Particle diameter d_p can be calculated by using the volume average. So, d_p essentially is given by the, 6 times the volume of the cylinder divided by pi, whole to the power of 1 by 3. Essentially, we are finding out what should be the diameter of an equivalent spherical particle which occupies the same volume as that of the cylinder. So, suppose let us say we sketch the cylinder here.

The diameter of the cylinder let us say D is = 0.25 centimetres. That is 0.25 centimetres. And the length of the, which is basically the length of the cylindrical catalyst pellet. That is essentially = 0.5 centimetres. So now, how do we find this? What is the volume of the cylinder? We do know what the volume of the cylinder is. So, this is essentially given by 6 into pi D square by 4 into the length of the cylindrical particle divided by pi to the power of 1 by 3.

So, we can now substitute these numbers. So, that will, so pi will cancel out. So, it will essentially be 6 by 4 into 0.25 into 10 power - 2 square into 0.5 into 10 power - 2. That raised to the power of 1 by 3. So, that is essentially = 3.61 into 10 power - 3 metres. So, the equivalent particle diameter for the cylindrical catalyst pellet that is actually considered in this problem, is given by 3.61 into 10 power - 3.

So, what we will see from the next class is we will take forward from the equivalent particle diameter we estimated from here. And we will look at the other parameters, estimate the other dimensionless quantities. And we will find out what is the mass transport coefficient using the Thoenes-Kramer correlation method and estimate the conversion. Further, we will go

ahead and look at the Colburn J D factor correlation method. And we will estimate the conversion based on that method as well. And we will compare the conversions estimated based on both these methods. Thank you.