Chemical Reaction Engineering - II
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Lecture – 42
Fluidized Bed Reactor Design IV

Then let us look at the mass transport between bubble and cloud.

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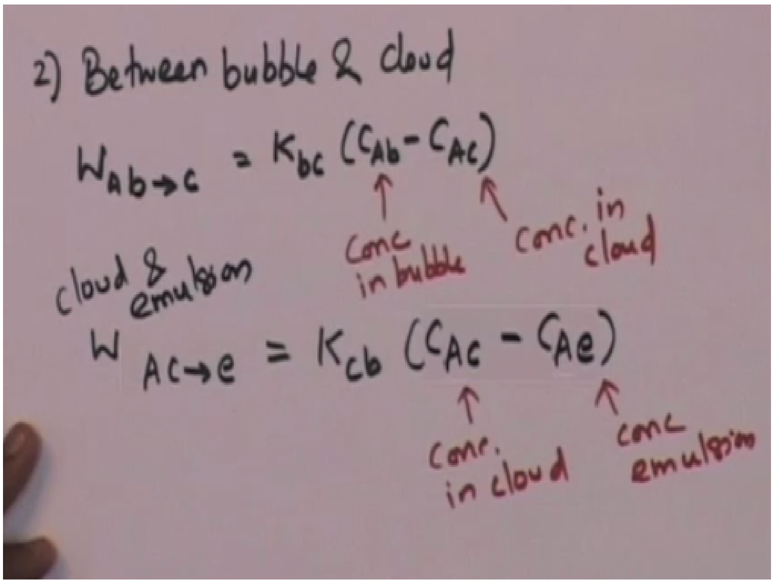

So suppose if the, so let us first look at the transport of the reactant from the bubble to the cloud. So, suppose if A is the reactant, so the flux at which the species A is being transported from the bubble to the cloud, flux at which it is transported is actually given by the mass transport coefficient Kbc * C Ab – C Ac, where C Ab is basically the concentration. So that is the concentration of the species in the bubble phase and this is the concentration in the cloud phase.

So this expression provides the flux at which the species is being transported from the bubble phase to the cloud phase and similarly for transport from the cloud phase to the emulsion phase, the expression can be written as K cb where J cb is the corresponding mass transport coefficient and the previous case there K bc is the corresponding mass transport coefficient multiplied by C Ac – C Ae where C Ac is the concentration of species A.

So C Ac in the cloud phase and this is the concentration of species in the emulsion phase. So this is for the mass transport between the cloud phase and the emulsion phase. So similarly one can actually write similar transport for the product species which is being transported back from the emulsion phase back into the cloud phase and back into the bubble phase. So Kunii Levenspiel, once again they have developed a correlation in order to find out what these mass transport coefficients are.

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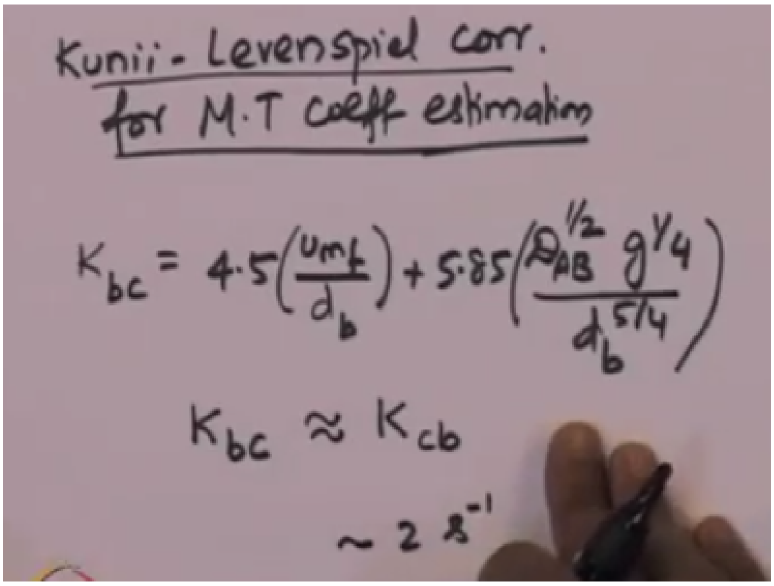

So they have developed a correlation for estimating these mass transport coefficient and so that is given by K bc which is the mass transport coefficient for reactant species to go from, for species to go from the bubble phase into the cloud phase and that is given by 4.5 * the minimum fluidization velocity umf/the diameter of the bubble + 5.85 * the diffusivity D AB to the power of 1/2 * gravity to the power of 1/4 / the diameter of the bubble to the power of 5/4.

So that is the correlation which provides an estimate of what is the mass transport coefficient between the bubble phase and the cloud phase. Now because the mass transport actually occurs by the exchange of volume between the cloud phase and the bubble phase one could assume that the mass transport between the mass transport coefficient for transport from the bubble through the cloud phase should be approximately equal to the mass transport coefficient from the cloud phase back into the bubble phase.

And typically the order of magnitude of this mass transport coefficient is of order of 2 second -1. Remember that K cb is a mass transport coefficient. So now let us look at the correlations for cloud 2 emulsion.

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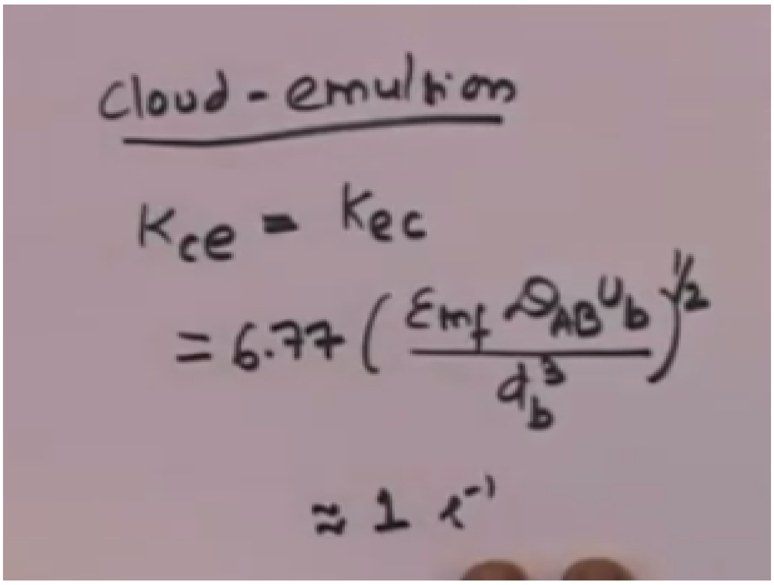

Mass transport from cloud to the emulsion and that is typically given by K ce + K ec that is the Kce is the mass transport coefficient for transport from the cloud phase to the emulsion phase and K ec is the transport of products let us say from the emulsion phase back into a cloud phase and so that is given by the correlation 6.77 * epsilon mf which is the porosity at the minimum fluidization velocity multiplied by the diffusivity D AB into the velocity of the raising bubble divided by the diameter of the bubble to the power of 3.

Cube of that to the power of 1/2 square root of the whole expression and this is typically of the order of 1 second -1. So that is the order of magnitude of the mass transport coefficient. So let us next look at the reaction in the fixed fluidized bed reactor. Remember there are 3 factors which are controlling, one is the mass transport of the reactant species from the bubble phase into the into the cloud and into the emulsion in order for it to get in contact with the catalytic particles.

And then the next step is the reaction which is actually occurring inside the catalytic sites to form the product catalytic reaction which is happening inside the catalyst site to form the products and once the products are formed they are transported back into the bubble phase. So let us look at the reaction in the fluidized bed reactor.

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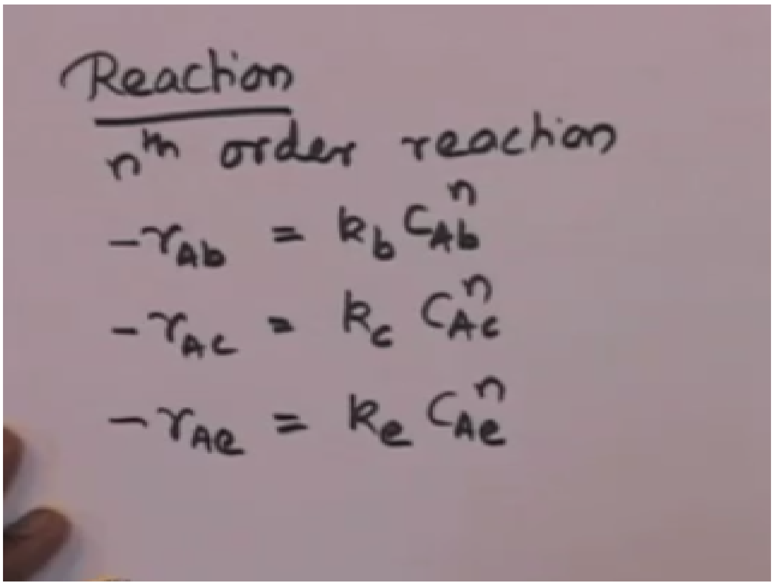

Let us look at the reaction, so suppose if it is an nth order reaction, suppose if it is an nth order reaction then the reaction rate in the bubble phase can actually be given as Kb * C Ab to the power of n, so that is the bubble phase and similarly for the cloud phase it can be given as Kc * CAc to the power of n where Kb and Kc are the corresponding rate constants and then for the emulsion phase it can be written as Ke * C Ae to the power of n.

Where the C Ab is the concentration of the species in the bubble phase and C Ac is the concentration of the species in the cloud phase and C Ae is the concentration of species in the emulsion phase. Now it is important to write these rate expressions in all 3 phases although the emulsion phase actually contains the maximum number of particles. The bubble phase and the cloud phase also will have some particles.

And therefore it is important to write these expressions because the reaction can in principle occur in the catalyst particles in each of these phases. So now next we can write a mole balance, once we know the reaction rates we can now write a mole balance in the fluidized bed reactor in order to capture the behavior of the concentration of the reactant species in the reactor.

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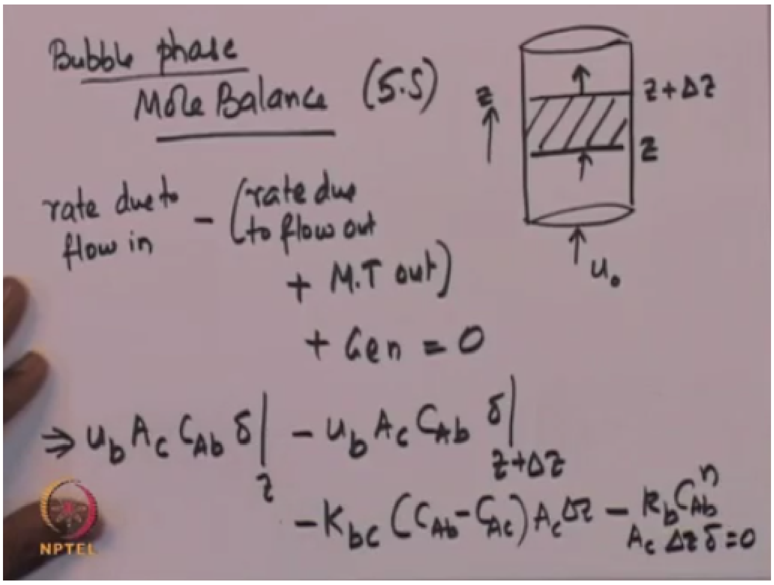

So now let us consider a small element, let us consider a fluid as bed reactor and if let us say that the fluid is entering at a superficial velocity of U0 and then there is a small element between Z and Z+ delta Z and if we assume that the upward motion or the direction of the fluid flow is the positive direction then we can now write a mole balance for the bubble phase.

You can now write a mole balance for the bubble phase which is basically rate due to flow into the bubble phase - the rate with which the fluid stream leaves because of flow + the rate at which the fluid species is actually leaving the bubble phase because of mass transport + whatever is being generated that should be = 0, under a steady state condition. So if we assume a steady state condition then this is the mole balance.

So now when we plug in all the corresponding expressions, rate due to flow that is into the bubble phase is given by the velocity of the bubble Ub * corresponding cross section Ac * concentration of the species in the bubble phase * delta. So delta is basically the fraction of the bed that is actually in the bubble phase and that at that particular location Z that is the rate at which the species is entering this small element in the bubble phase.

And then the rate at which the species is leaving in the bubble phase at Z + delta Z is given by Ub Ac C Ab * delta at Z + delta Z and the mass transport is given by - K bc * C Ab that is the concentration of the species in the bubble phase - the concentration of species in the cloud phase * cross section area * delta Z. So that is the rate at which the species is actually leaving the bubble phase and going into the cloud phase - the corresponding reaction rate.

So that is Kb, if the Kb is the reaction rate constant * C Ab to the power of n, so that is the C Ab is the concentration of species in the bubble phase * the cross section * delta Z * delta, so that should be = 0. So that is the mole balance for these species in the bubble phase. So now we can rewrite this mole balance as by taking a limit that.

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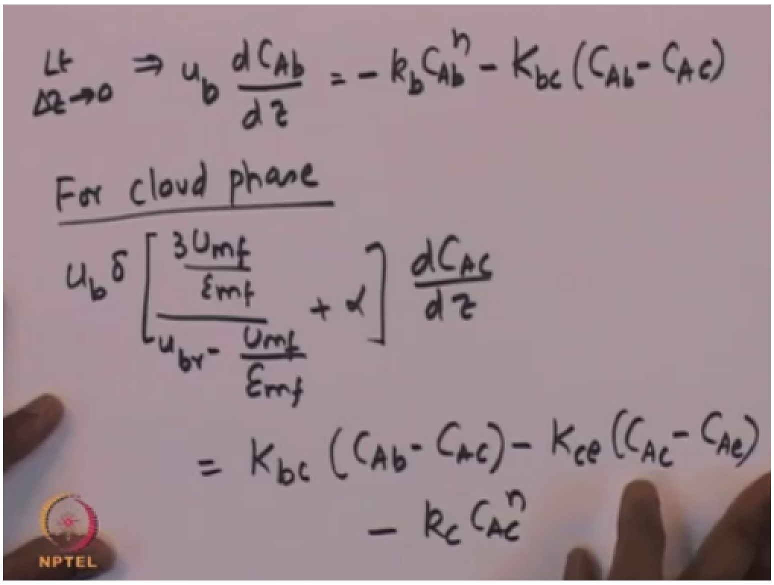

So by taking limit that delta Z goes to 0. We can rewrite this model as Ub which is the velocity with which the bubble is racing inside the fluidized bed reactor into dCAb/dz that should be = - kb C Ab to the power of n – Kbc which is the mass transport coefficient between the bubble and the cloud phase * C Ab – CAc. So that is the model, the mole balance for the bubble phase.

So similarly for the cloud phase, the mole balance is given by Ub * delta * 3 times Umf, a very similar balance can be written and taking the limits of delta Z going to 0, one would get that the expression for a mole balance for the concentration of the species in the cloud phase is basically given by this expression here * dC Ac/dz, that should be = the mass transport coefficient of the species from the bubble to the cloud phase.

That is basically added into the cloud phase * CAb – CAc- Kce that is the mass transport coefficient for transport of the species from the cloud phase into the emulsion phase that is given by CAc - CAe - Kc which is the rate constant for the reaction if the catalytic reaction is happening in the catalyst particles which may be present in the cloud phase. So that is the mole balance for the cloud phase.

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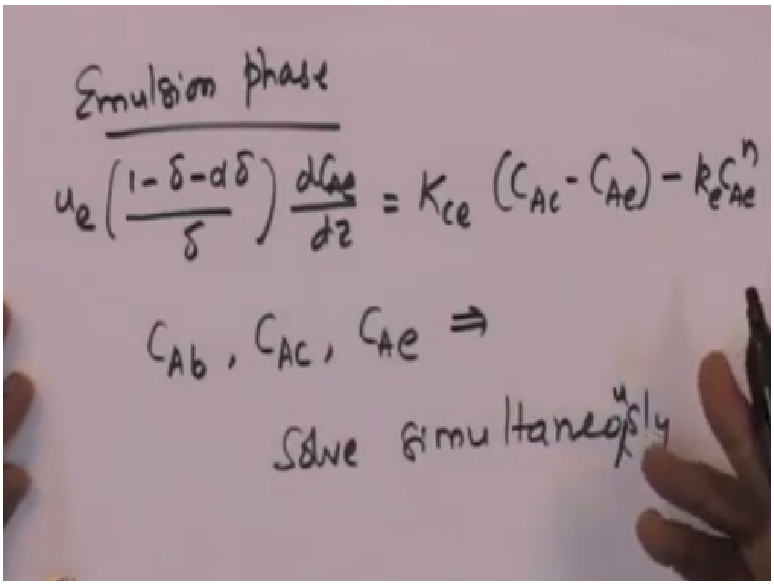

And then the mole balance for the emulsion phase is given by, for the emulsion phase that is given by Ue which is the velocity with which the emulsion phase is wing * 1- delta - alpha * delta/delta * dC Ae/dz that should be = the mass transport coefficient between the cloud and the emulsion phase * C Ac – C Ae - the rate at which the species is actually being consumed because of the reaction that may be happening in the emulsion phase.

So if we need to find out what is the concentration of the species in the bubble phase in the cloud phase and the emulsion phase then these 3 equations have to be solved simultaneously. So these things have to be solved simultaneously. So once we solve them simultaneously then we can find out the expression for C Ab, C Ac and C Ae, what is it is relationship? how the profile changes with respect to the position inside the fluidized bed reactor.

As this is a non-linear equation it cannot be solved analytically and one has to resort to numerical techniques to solve these set of equations; however, if we make an assumption that the reaction is a first-order reaction.

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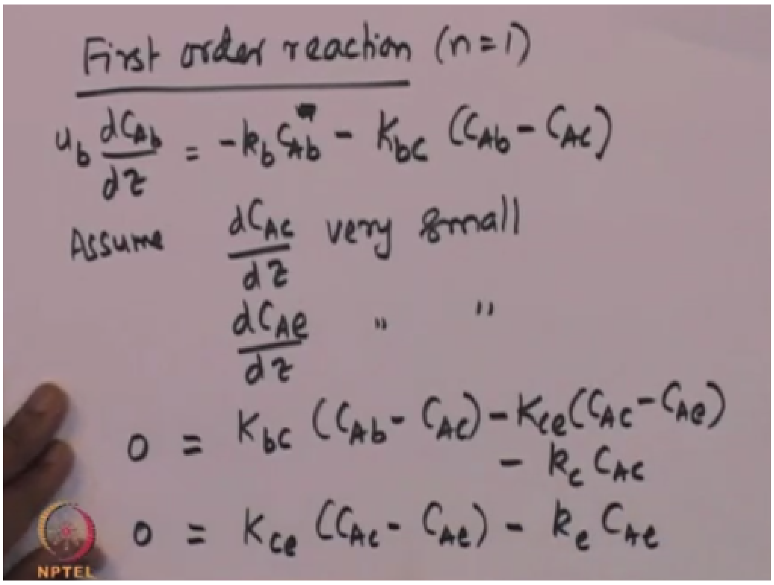

Suppose if we assume that it is a first-order reaction. Suppose if the reaction the catalytic reaction which is happening is a first-order reaction then we can actually write the expression as Ub * dC Ab/dz that is = - kb * C Ab to the power of n - the mass transport coefficient Kbc * n=1 C Ab – C Ac and there are other, suppose if we assume that that dC Ac/dz, which is the rate of change of the concentration with respect to position the cloud phase, if this is very small.

And similarly if we assume that dC Ae/dz is also very small then we can write the model equations for these 2 concentrations as they basically become like this, where 0 = the mass transport coefficient Kbc * C Ab- C Ac – K ce * C Ac- C Ae – kc * C Ac and similarly for the emulsion phase the mole balance will become Kce * C Ac – C Ae – ke * C Ae. So that is the mole balance for the emulsion phase. Now because it is a catalytic reaction, so Kb, which is the corresponding rate constant.

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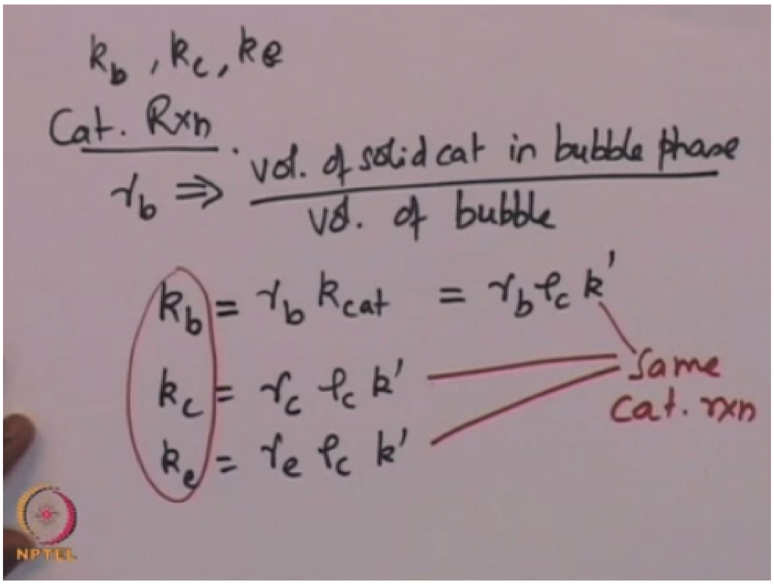

Suppose kb, kc and ke, these are the corresponding rate constants for the reaction, which is actually occurring in the bubble phase, cloud phase, and the emulsion phase respectively. So now suppose if it is a catalytic reaction and if gamma b is basically the ratio of volume of solid catalyst in the bubble phase/the volume of the bubble. So this provides an estimate of what fraction of the bubble volume is actually contained by the solid particles which are actually carried by the bubble phase.

So if we know this expression then we can actually rewrite the rate constant in terms of the intrinsic rates. So that will be = kb is given by gamma b, which is the fraction of the volume inside the bubble which is occupied by the solid particles carried by the bubbles * the corresponding reaction rate which is occurring in the catalysts surface of the particles and so now that can actually be rewritten as gamma b * rho c * k prime.

Where k prime is the gram mole that is reactor per unit weight of the catalyst per unit time and rho c is the corresponding density of the catalyst. So similarly we can actually write, we can write kc is basically = gamma c which is the volume of solid catalyst which is present fraction of volume of the cloud phase which is occupied by the solid catalyst that * rho c into k prime and similarly ke = gamma e * rho c * k prime.

So notice that the K prime is basically same because it is the same catalytic reaction, which is happening in the solid particles which are present in these 3 phases. The overall reaction rate is different in these 3 phases because the amount of catalyst particles which is present in each of these phases are different and therefore that is actually accounted for the overall reaction rate constant.

So now we need to estimate what is this gamma b, gamma c and gamma e are. So if we know that estimate then the mole balance can actually be solved.

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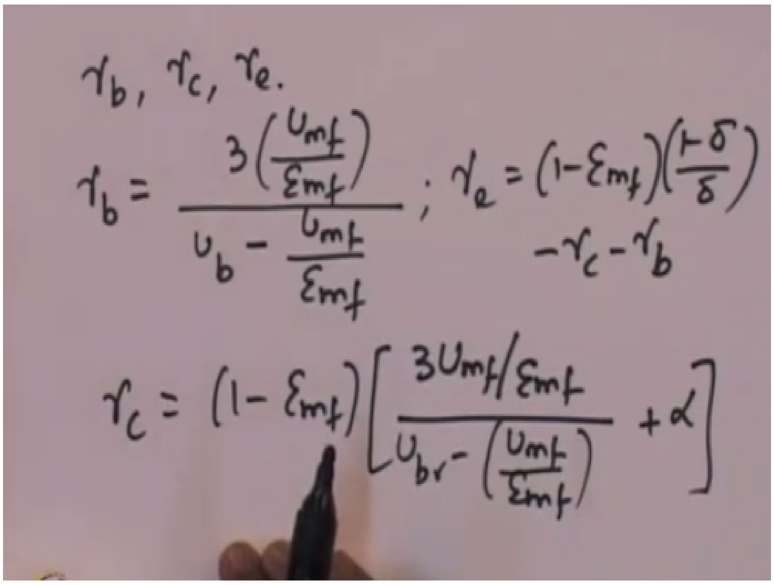

So we need to find out what is gamma b, gamma c and gamma e. So once we know this we can actually solve the model equation and so gamma b is essentially given by 3 * Umf/epsilon mf/ub – umf/epsilon mf and similarly gamma e is given by 1 - epsilon mf * 1 – delta/delta - gamma c - gamma b.

So that is gamma e is the fractional volume in the emulsion phase which is occupied by the solid catalyst and gamma b is the corresponding fractional volume in the bubble phase and gamma c is the fractional volume in the cloud phase occupied by the solid particles which will be 1 - epsilon mf * mf/epsilon mf/Ubr – Umf/epsilon mf + alpha.

So these things can be estimated simply by estimating in terms of the properties such as the porosity and the minimum fluidization velocity et cetera, what is the volume of the bubble and what is the fraction of the bubble which contains the solid particles, what is that volume. So once we estimate these volume and take the ratio, we can find out these expressions for the volume fractions in each of these respective phases that is contained by the solid particles.

So now if you know all these expressions, then we can now solve the model equations in order to find out the design parameters of the fluidized bed reactor. So the complete mole balance for the first-order reaction is basically the set of mole balance equations are.

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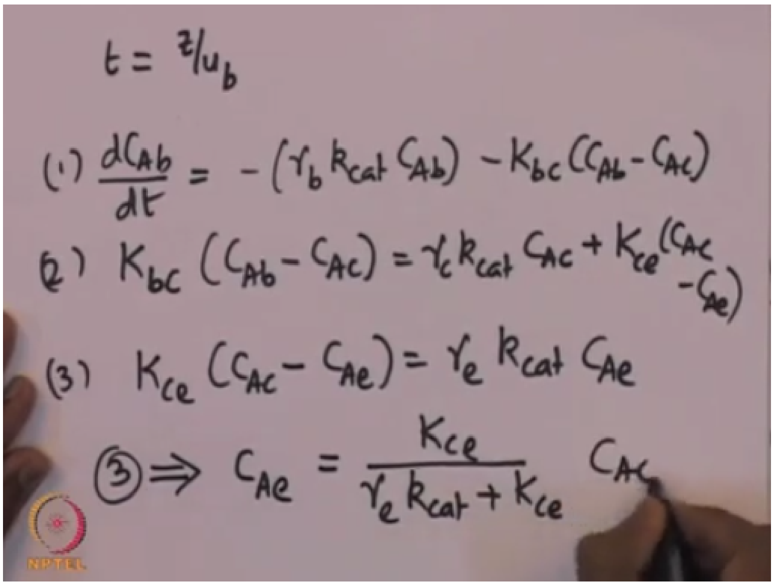

Suppose if we assume that the time is = z/ub, so remember that the time that is spent by the bubble inside the bed is actually an important parameter that controls the performance of the fluidized bed reactor. So t here refers to the time that is actually spent by the bubble inside the fluidized bed reactor till this position z. So ub where ub is basically the velocity with which the bubbles are actually rising inside the fluidized bed reactor.

So the mole balance will be d Cab/dt that is = - gamma b * into the specific rate constant for the catalytic reaction * C Ab - Kbc * C Ab – C Ac and the second equation is Kbc which is the mass transport coefficient between the bubble and the cloud phase that * C Ab – C Ac that should be = gamma c * the rate constant for the catalytic reaction * C Ac + the mass transport coefficient Kce * C Ac – C Ae.

And then the third equation would be Kce * C Ac – C Ae that should be = gamma e * the rate constant for the catalytic reaction * C Ae. So now if I look at the third equation, from third equation I can actually rearrange the third equation and find an expression for C Ae and that C Ae = Kce/gamma e * k catalyst which is the reaction rate constant for the catalytic reactions + Kce * C Ac.

So further rearrangement of the expressions can actually be performed in order to estimate what is the concentration of the species in the in the cloud.

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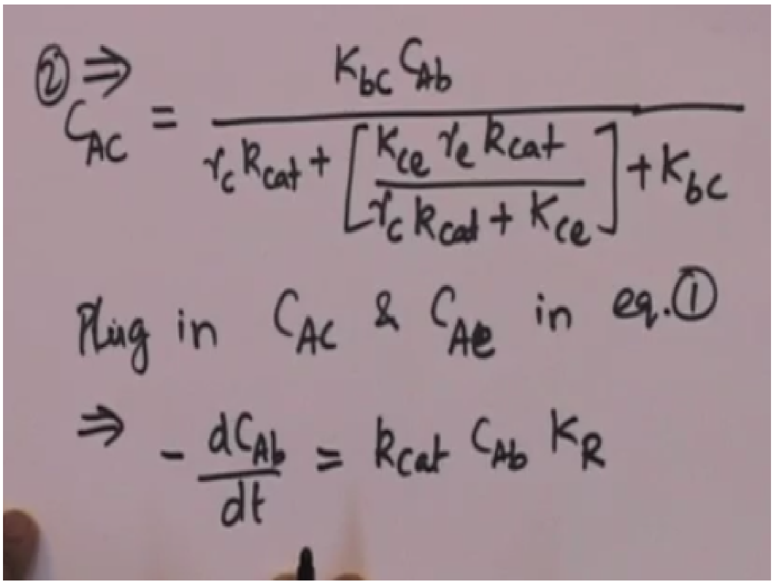

And that is from second equation we can find out, so substituting the expression for the concentration of the species in the emulsion phase * the mole balance expression for the concentration of the species in the cloud phase we can find out the expression for the concentration of the species in the cloud phase and that is given by Kbc * C Ab/gamma c * k catalyst + Kce * gamma e k catalyst/gamma c * k catalyst + Kce + Kbc, so that is the corresponding mass transport coefficient.

Now plugging in all these expressions into equation 1. So plug in expression for C Ac and C Ae in equation 1 we will get, so what we can find is that – dC Ab/dt that is = k cat * C Ab * some overall constant KR and this KR is essentially given by the overall constant KR is given by.

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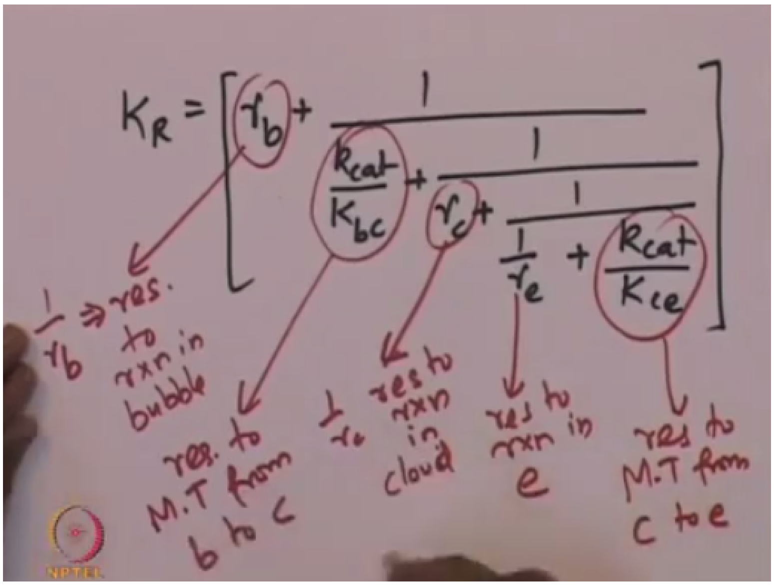

Gamma b + 1/k catalyst/Kbc + 1/gamma c + 1/ 1/gamma e + k catalyst/Kce. So that is the expression for the overall reaction rate and if I look at this expression gamma b, gamma b basically captures the 1/gamma b is the resistance for resistance to reaction in the bubble and k cat/Kbc is the resistance to mass transport from bubble to cloud and gamma c is resistance to 1/gamma c is resistance to reaction in the cloud phase and this is the resistance to reaction in the emulsion phase.

And this is the resistance to mass transport from the cloud to the emulsion phase. So there is overall constant essentially captures the resistances that is all the resistances that are actually present in this system. So now using the appropriate stoichiometry we can say that.

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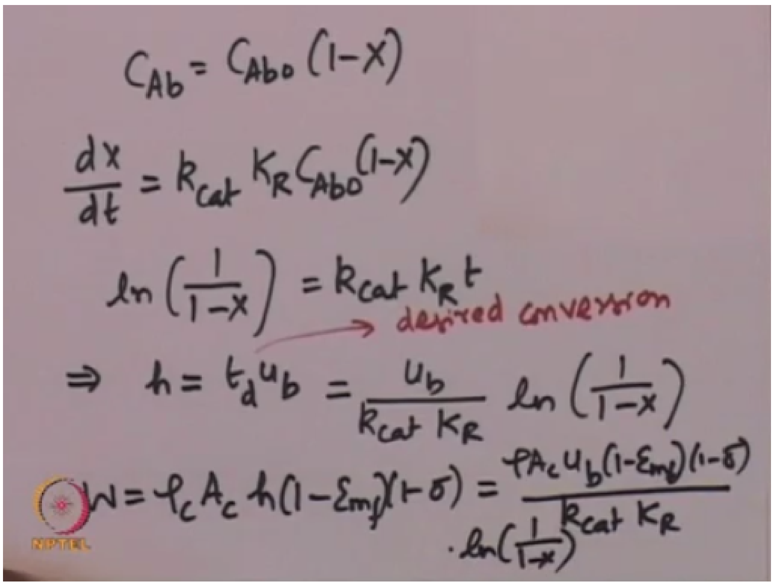

C Ab = C Ab0 * 1- X where C Ab0 is the concentration of the species at the inlet of the fluidized bed reactor and so we can now rewrite the mole balance as dx/dt = k cat * KR, that is the overall rate constant which captures all the resistances which are involved * 1- X. So now we can solve this equation and you can find that lon of 1/1-X that is = k cat * KR * t. So this provides the relationship between the conversion as a function of the time that is actually spent by the raising bubble inside the fluidized bed reactor.

So from this we can find out what is the overall height that is required. So that is = t * ub and that is the height that is required for, suppose if a specific conversion is set what should be the conversion supposing if for a desired conversion if td is the time that is required from this expression for the desired conversion. So this corresponds to the desired conversion. If this corresponds to the time for the desired conversion, then the height of the bed can actually be estimated by using this expression td * ub and that is = ub/k cat * KR * lon of 1/1-X.

And from here we can find out what is the weight of the catalyst that is given by rho c Ac * h * 1- epsilon mf * 1- delta. So that is given by rho Ac ub * 1- epsilon mf * 1 – delta/k cat * KR * lon of 1/1-X. So that is the expression for the weight of the catalyst. So let us quickly just rewrite the rate of expression for the weight of the catalyst.

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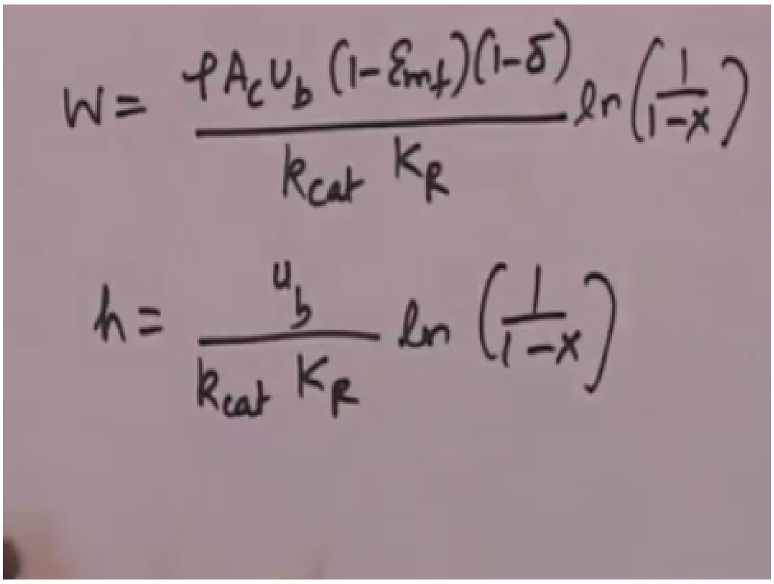

So that is given by rho Ac ub * 1- epsilon mf * 1- delta/k cat * KR which captures the which is basically the reflects the overall resistance * lon of 1/1 –X and the height which is required for the bed which is an important design parameter is basically ub/k cat*KR * lon of 1/1-X.

So let us summarize what we have learnt in this lecture. So what we have seen is we have actually designed a fluidized bed reactor.

We started by looking at various parameters estimating the various parameters which is required to design a fluidized bed reactors for example what is the, how to estimate the velocity of the raising bubble, how to estimate what is the fraction of the bed that is actually occupied by the bubbles et cetera and then we found out what is the rate law that corresponds to the catalytic reaction that is happening in the particles which may be present in the bubble or cloud or the emulsion phase in any of these 3 phases.

And then we looked at the mole balance for the species in each of these phases which incorporated the transport of species from the bubble phase to the cloud phase and cloud phase to the emulsion and using this mole balance we actually assumed that it is a first-order reaction and found out what are the important design parameters such as the height of the fluid as bed and weight of the catalyst which is required for a given conversion to be achieved using a fluidized bed reactor. Thank you.