Environment Engineering: Chemical Processes
Prof.Dr. Bhanu Prakash Vellanki
Department of Civil Engineering
Indian Institute of Technology – Roorkee

Module No # 03
Lecture No # 12
Material Balance for Reversible Reaction

Hello everyone welcome back to electric session I guess right so we have been again talking about kinetics and application of mass balances to the various reactors. So as you are have been following with course I guess you know have been spending considerable time on this particular aspect and reason being that the application are (()) (00:43) and you know wherever you work I guess right you are going to if you derive into the details going to apply material balance on most of the reactors that you see here.

So again we have been looking at I believe an irreversible reaction case A goes to 2B and so on so now we are going to make it slightly more complex A goes to B with this time it is irreversible reactions B also transforms to A right. So let us look at the particular example I guess.

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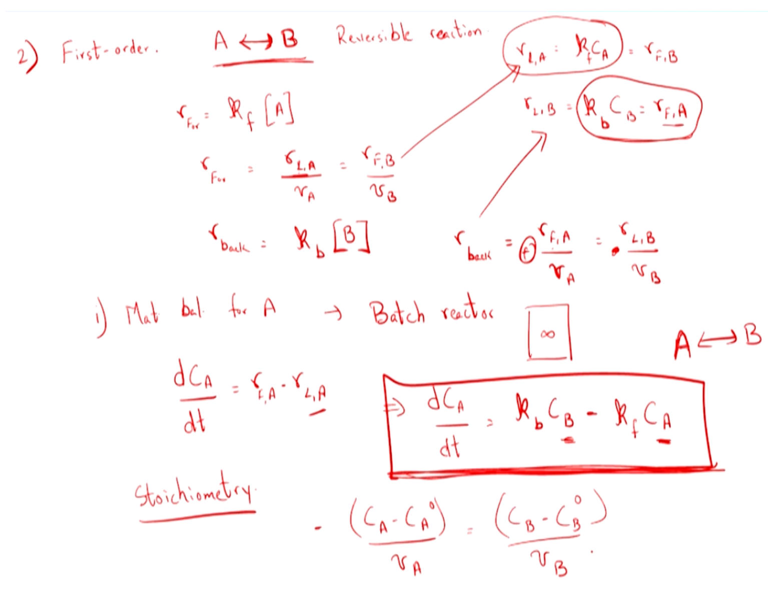

So what do we have here now we have a first order right and instead of just being A goes to B or A goes to 2B as in the earlier case we are also going to have a reversible reaction so this is now a reversible reaction right. So what is next let us identify rate of loss of A rate of loss of A = rate constant into concentration of A right and that will again be = rate of formation of B right so that is something that obvious here and what is rate of loss of B that is going to be equal to now we have a K again.

So let us call this K forward the earlier case and this as K backward right rate constant for backward reaction and that is going to be CB and that is again going to be = rate of formation of A I mean this is not clear let us clear this up I guess what I rate of reaction 1 reaction 1 is the forward reaction what is that equal to it is the rate constant we say rate constant is K forward right and times the reactants what is the reactants for the reaction going forward it is concentration of A right so that is what we have here.

And for this particular reaction we know that you know rate of what we say let us say forward I will call this forward rate of forward will be equal to rate of 1 / or rate of loss of A right and this case by the stoichiometric coefficient will be equal to rate of formation of B by the stoichiometric coefficient of B and I believe that is what we see in this particular case here and say if we are talking about rate of the backward reaction right.

And here it is going to be equal to rate constant of backward reaction times the concentration of the reactants and in this case we are talking about the backward reaction right so that reactant is B right and as we are aware how do we set them up to the other aspects here the rate of the backward reaction is going to be equal to rate of formation of A right as we see B goes to A / stoichiometric coefficient of A right and that is equal to rate of loss of B anymore sign here right.

If I did not use the terms loss or formation then I obviously need to put in the relevant sign with respect to negative and positive for formation or loss. So now let us move on we will have out material balance for our A material balance for A so our case now obviously is the first case always out batch reactants we are looking at our batch reactor and again what is that it is a close resistant with now flow coming in and going out and obviously it is completely mixed throughout.

And we know that for the batch reactor it is at the relevant equation the mass balance is DCA. DT = rate of formation of A – rate of loss of A right and reason for choosing this example where

A goes to B and B geos to A or it is A and B are reversible I guess the transformation of A and B is that now I have a new term to unlike the lass case which is the loss of A.

So let us plug in the relevant values and see what we have so I believe that would transform into DCA / DT would be equal to rate of formation of A here please and that is here rate of formation of A right that is equal to KB CB and – and where is the rate of loss of A and that is somewhere out here and that is going to be equal to rate constant of the forward reaction into concentration of A.

So as we see here we are now left with a dilemma here and the reason being that we have one equation here and we have 1 unknown here unlike the last case where were able to integrate that because we had only one particular variable there that here we have two variable so how do we go about that again so we end calculating the DCA/ DT here right and as we were just discussing we have two variables here and we have thus not able to solve this particular equations by itself so what do we do?

We end up applying stoichiometry and let us look at what we have their so we have change in ACA – A naught / stoichiometry coefficient of A and this is going to be let us say negative I guess times CB BC naught by stoichiometric coefficient of B right.

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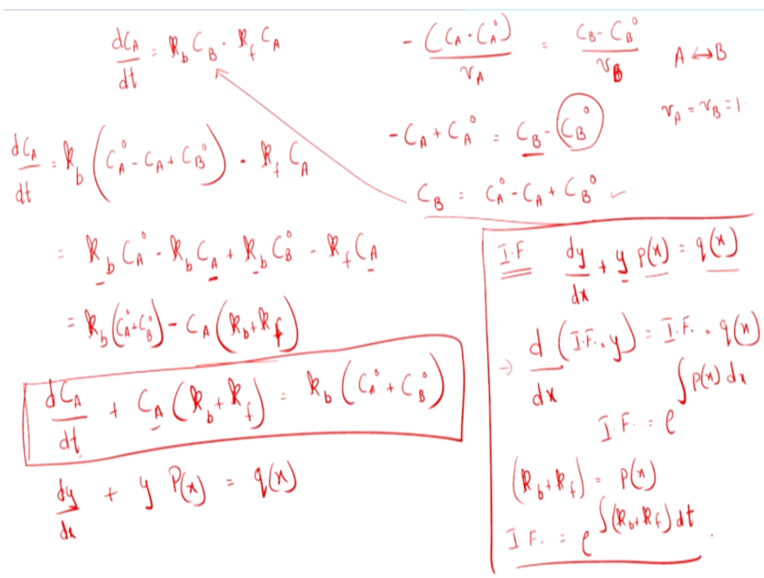

So let me just drag this down in next page it is DCA / DT = KBCB right constant of B into concentration of B – KF into concentration of A and we at the same time stoichiometric we have ACA – CA naught by the negative symbol we are going to move in the opposite direction stoichiometric coefficient of A pardon me = CB – CB naught by stoichiometric of A right.

So this is what we have pardon me not A here it is going to be B right and we know that for this reversible reaction A goes to B stoichiometric coefficient of A as going to be equal to the stoichiometric coefficient of B that is equal to 1. So let us see what we end up adding here I guess substituting that – CA + CA naught = CB – CB naught right and what do we see here I want to calculate for CB so CB is going to be = CA naught – CA right and if I take term out to the left hand side it is going to be + CB naught.

So let us look at our calculation right CB is going to = CA naught – CA + CB naught right it is in the white track here and I am going to plug this equation in here right and let us see how this going to transform into DCA / DT = the rate constant of backward reaction times CA naught – CA + CB naught right – KF into concentration of A right and so that where then KB into CA naught – KB into CA + KB into CB naught – KF into concentration of A that here will be what now please I am going to take – CA a common here guess – CA into KB + KF right.

And here I can going to be KB common factor here KB into CA naught + CB naught right so this what we have here let us check out calculations here pardon me so CA – CA common KB + KF and that is what we have here and then we have KB the common factor here and CA naught + CB naught right. So I guess let us realign this so that it is similar to what it is that we have look at in you know similar cases in the path let us say + CA into KB + KF = KB into what we have here CA naught + CB naught right.

So now how do we solve this I guess right and this is the equation we have and we have struck with here. How do we end up solving this? So for this case I believe we need to use the integrating factor right. And what is the about? I guess most people have the background of those do not have this we are going to look at this so if your differential equation of this particular form DY / DX + Y into P of X = Q of X right.

So differentiation of Y with respect to X + Y times function of X many function = A times the function of X so what do we see here though. So DY is your CA here X is your T so DCA / DT + CA which is Y term here right or let me write that down here I guess so it makes more sense so DY / DX + Y times of function of X = Q times function of X right that is what we see so DY / DX + Y times the function of X = Q times function of X again right.

For that case what is the solution of where get that from I get that from DY / DX of introduce the term integrating the factor Y into Y = integration factor into Q of X right and what is that integrating factor about right that is = E to the power of exponential of P of X into TX right so would be of solution obviously once we integrate this will get the solution so in our case what is the P of X please in our case the P of X is KB + KF that is our P of X right.

And so our integrating factor in this case it is going to be E to the power of Kb + KF times what is our X is RT DT right so what do we have integrating factor as this so let us write this down in the second page and the continue from their please.

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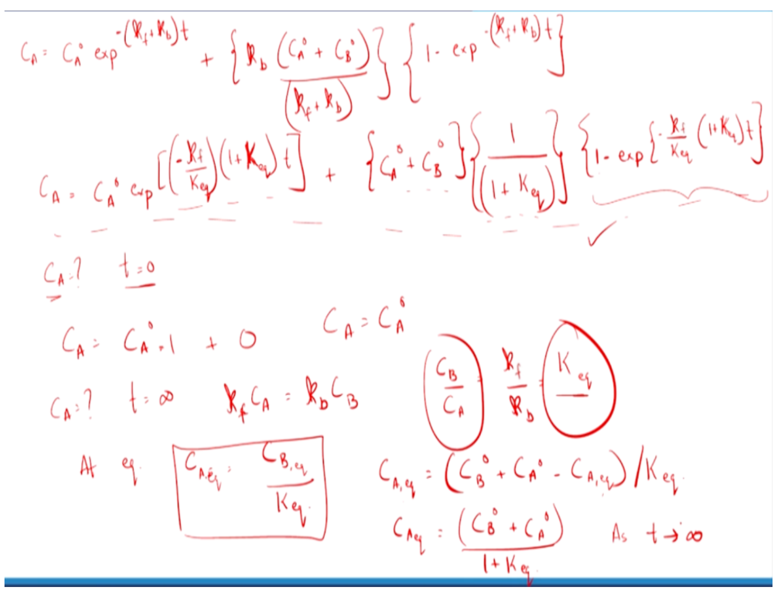

So we just have integrating factor = exponential of P of X that is in our case KF + KB times DX and that is for us DT I guess right is not that the case please that is our case here what is that DC / DT and the equation is something like DCA / DT + CA into KF + KB right was = KB times concentrations of A initial and concentration of B initial so this is what we have right as we just talked about we have our solution here.

So without trying to you know take you through the relevant details right we will have the relevant solutions here so that looks like should end up as being CA = CA naught into exponential of – KA + KB into time K not KA pardon me CAKF + KB into CA naught + CB naught right by KA + KB right and hopefully we are in the right track similar into 1 – and this I guess it is constant right exponential of into time so this is our solution to our equation now.

And where is this from once we identify the method to be the one who get if you use to integrating factor so right let us say what we have here. So before we go further obviously we have to check right so before we check let us simply this bit further and then go by so I want to apply within or take out KF right the rate constant in the backward constant anyway and have only K forward and K equilibrium rate constant and equilibrium constant.

What is KF? Rate constant and the forward reaction KB is the rate constant of the backward reaction and what is K equilibrium obviously it is the equilibrium constant right so at equilibrium let us say at equilibrium what is going to be now you know that rate of forward reaction is equal to the rate of the backward so what was that translate into.

So that is KF into CA = KB into CB or what is this mean? It means CA / CB = CA / CB = KB / KF right so what is that equal to it is 1 / K equilibrium right and that is what you would see or let us write down in another matter and to the form how do get this K equilibrium now. For A goes to B now what is that we know it is CB / CA right that what we get these particular this particular from and that is equal to CB / CA = KF / KB right so let us plug this into relevant equation.

And so what do we end up with here I guess so we have CA = CA naught into exponential of – KF + KB into time + KB into what else we have here CA naught + CB naught / KF + KB right into 1 – exponential – KF + KB into time this is what we have now we plug in the relevant equations what did they transform into CA = CA naught into exponential – KF / K equilibrium and this is 1 particular term into 1 + K equilibrium into obviously time again and that is what we have here earlier right + CA naught + CB naught right times K CA naught + CB naught.

And we early now I have KB / KF + KB let us see what that transform into that would transform into 1 / 1 + K equilibrium right into 1 – exponential – KF / K equilibrium it should be similar to what we have here right into 1 + K equilibrium K is the capital K obviously right K equilibrium times T anyway it is complex equation obviously we do no expect it to bring it up but the particular reason why we just try to solve for this and we will see why I guess right.

So here we are going to check for our limits and what are they and we are going to look at what is going to be CA right when time = 0 right what is CA going to be time – 0 so let us club that increase and look that up. So CA will be equal to CA naught right and what do we have here times 0 T to the power of 0 right and that is going to be = 1yes + CA naught CB naught and here more or less all this same stay the same 1 – E to the power of 0 so all these term here become 0 and T = 0.

So that means = 0 as you see just simply into CA = CA naught that means the solution is right yes so that is what we expect here and that is what we see too right. So let us see what the system would or what is this A or equilibrium value going to B and time goes to infinity right again at infinity we go that what is that guess KA CA or KF CA = K backward into CB so what was that mean again CB / CA this is something we just discuss the value = rate of constant of F/ rate constant of B that = the equilibrium right.

So at equilibrium what do we see here CA at equilibrium right CA at equilibrium = CB at equilibrium this is from this equation here right CB at equilibrium by K at equilibrium yes and so this is we have until now so let us say if this is something with that we can use and go through I guess and what next please we have CA at equilibrium = we know CB at equilibrium is going to be what now BC naught + CA naught –CA at equilibrium right divided by the equilibrium constant K EQ.

So again CA at equilibrium is now going to be what now CB naught + CA naught right and as you see then transform into by 1 + K equilibrium yes and that is what we see here CA take this out here and that becomes we are on the right track here yes and T goes to infinity I guess right as at T goes to infinity what is that we expect that guess right as T goes to infinity let us see what happens now.

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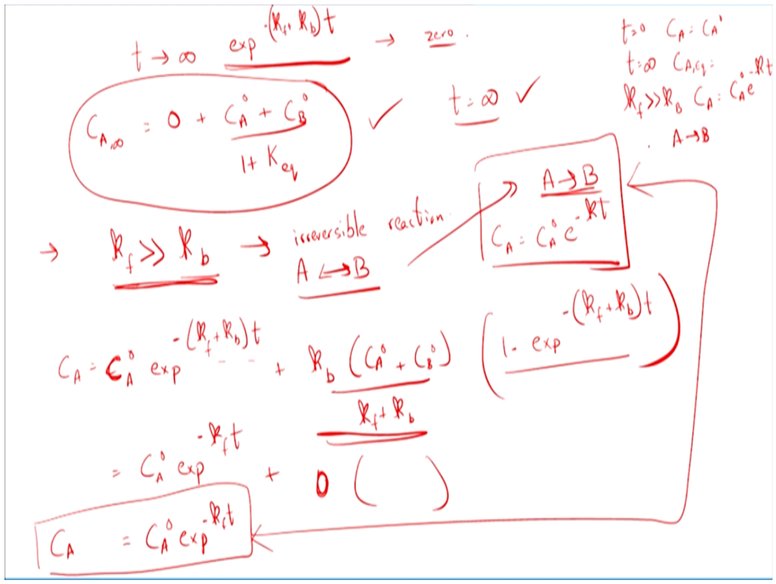

So we know that as T goes to infinity exponential – KF + KB into time this what we have in one of the equations right what will this go to this will go to 0 right this will go to 0 and then CA at infinity = what 0 so I am now take you through this particular equation here right so I am not plugging in time = infinity right so this term = 0 yes so this term will be 0 here and what else F again this term here is also 0 yes these two term converted to be 0.

So am I left with only left with these particular term and what is that is equal to 0 + CA naught + CB naught / 1 + K equilibrium right and that is what we just derived here and say again here that is the check again right so at time = infinity we just saw that the check was fine again so we looked at that so now look at the last case and we done with today. So we are going to look at the rate constant of the forward reaction is far greater than the rate constant of rate reaction what does this mean.

It means it is a irreversible reaction right let us plug this in and see what it is and if we look at that we also looked at I think in some cases A goes to B this is more or less irreversible reaction and we know that particular case CA was = CA naught into E power – KT right so we want to able to substitute the KF is far greater than KB in our reversible reaction transforming it into an irreversible reaction as A goes to B see if you get the relevant equation now right.

So if you plug it out and in this particular equation again this let us see what will end up with so we are going to have CA = CA naught into exponential of – KF + KB into T right + KB into CA naught + CB naught / KF + KB right hopefully we are on the right track into 1 – exponential of – what do we have here KF + KB into T right and so again we find this further we end up with CA naught into exponential of – K forward is far greater than K backward so it is just going to be K forward into time + right F we end with 1 – this term here going to then be 0 right.

This is going to be 0 into 1 – an so on this term so this is going to be this term here so as you see here we end with CA = CA naught into exponential –KF into time and what do we see here that is equation right is similar to what we just derived in previous session for goes to B right. So we just looked at the three cases where time = 0 we saw that CA = CA naught right and we also looked at the case when time = infinity CA at equilibrium we derived that and we also saw when K forward is far greater than KB right.

That the solution is similar to case when A goes to B when which is CA = CA naught into E power – KT right. So with that I guess we will be done for this session and thank you.