Environment Engineering: Chemical Processes

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Module No # 03
Lecture No # 11
Material Balance for Complex Reactors

Hello everyone so welcome back to our next lecture session so I believe we were talking about kinetics right and we were talking about rates of the reactions and how they depend upon the concentration of relevant reactants and then we discussed how temperature effects the rate constants I guess right we looked at linear equation and then we started discussing the mass balance equation and we also talked about the different or three kinds of reactors the batch reactors the plug flow reactors and the continuously stir tank reactor.

So we will have a very brief review about very mass balance and it is application to the batch plug flow and CSTR ad then we are going to move to the some of the applications I guess right so let us have a look at what we have been discussing.

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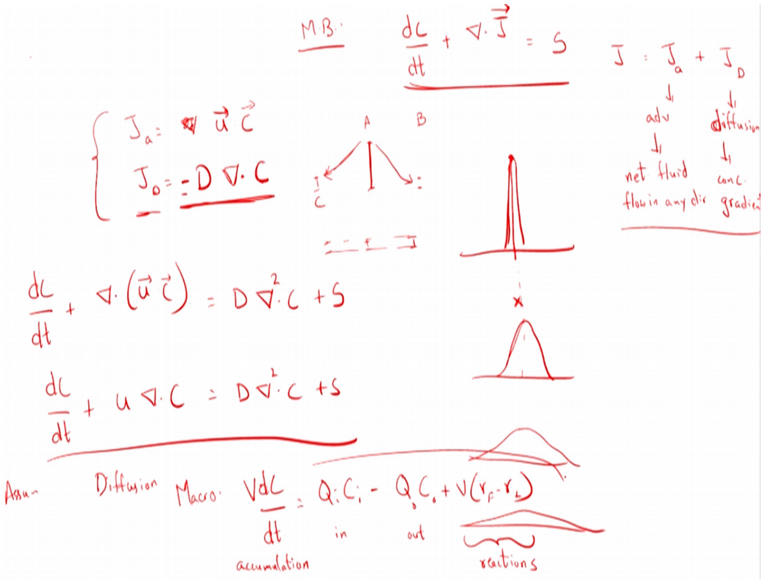

So we have been discussing about mass balance right and fundamental equation what is that I guess DC / DT + the del part of the flux is the vector here right = to the sources and sink and again the flux we have the two fluxes here 1 due to advection and 1 due to diffusion advection when you have net fluid flow in direction or in any direction right we talked about that and this is flux due to diffusion.

And in general driven by concentration gradient and this is what we have discussed so and the flux due to advection which said it is going to be = to what now pardon me right and this is what we have here and due to diffusion is going to be diffusion coefficient and the del product into C so substituting the relevant and here is going to be negative and why is that let us say the diffusion is such that it always drives or tries to minimize the gradient in concentration.

So the concentration is higher here and lower here the compound would move from .A to .B again random motion here if it is B here is going to move in these directions right random motions that after certain time you are going to have concentration at the same what do we say levels throughout let us say I think I will try to have a better representation here.

So let us say initially all my concentration is right here right at let us say X this is X distance X and this is my concentration peak here let us say initially right so with diffusion what starts happening I guess peak right at this point X it is going to start flattening out right. So finally we are going to have something like this and so on.

So this more or less due to diffusion it is going to be same in all the directions its random and it is also relevant I mean relevant diffusion equation is going to be the negative obviously because it is going to decrease and then the diffusion coefficient in dealt product of the concentration let us say so once we plugged these values back in our main mass balance equation what do we end up having please so DC/ DT + the del product of C let us say C is also gradient let us say = D del square C + source and sins.

And if I assume is at the velocity let us say DC / DT + U del. C = D del square C + source or sins right and this is what we discussed and the same manner we end up simplifying this equation when there is not diffusion and there is no diffusion or assuming that there is no diffusion let us say and then simplifying it further in the macroscopic level and macro level what do we have I guess we have V DC/ DT = Q in C in this is coming in this is Q out C out right going out + volume into rate of formation – rate of loss this is the one that looks at the relevant reaction right.

And this is what we have and this is the accumulation term and this is obviously being negative depending upon these factors here right and we discussed this particular aspect and we then applied them to three different kinds of reactors.

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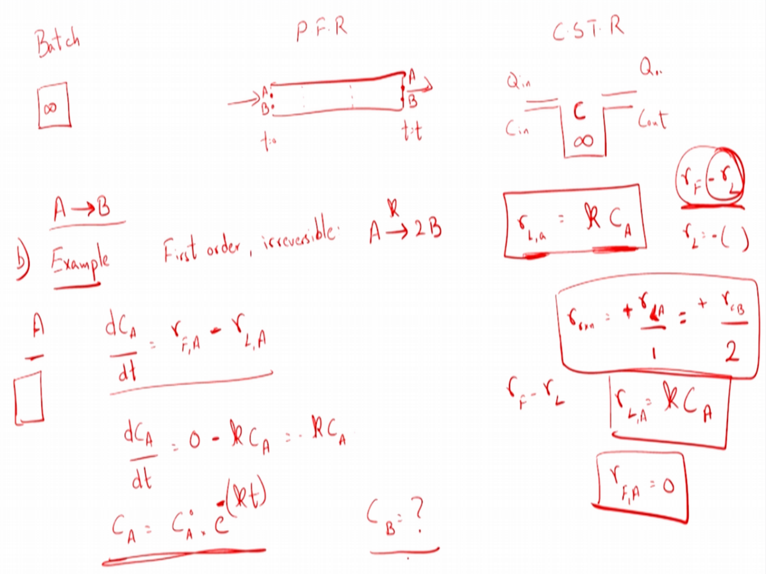

I believe they are batch and what else please plug flow reactors and what else please CSTR right and batch reactor no flow coming in or going out right plug flow rector flow through plug or flow through pipe let us say right and compounds coming in at same time will obviously go in but R definition exist at the same time right this and so on CSTR obviously I guess we have flow coming in we have flow going out and we have continuous mixing here and the concentration of relevant compound here.

And I believe we looked at the relevant derivation so we are not going to go into detail so and then we believe start talking about a particular example I believe it was A goes to B right that was with respect to batch reactor and I think we looked at CT = C naught goes to E power KT and so on so next we are going to come up with the another type of example and this example now we are going to look at is obviously again first order or we are going to start with baby steps.

First order irreversible right but to mix up or let us say to make it say slightly more difficult so then looking at A goes to B we are going to look at A goes to 2 B right and obviously here let us write down rate of loss of A and that is going to be equal to rate constant of this particular which is let us say K times concentration of A right and we are all aware that rate of particular reaction and thus the rate of loss in those particular compound always depends upon the reactants and not the products right that is why we have rate of loss = K CA or if you want to relate that the rate of reaction.

How do we do that? Rate of reaction = rate of loss of A by the stoichiometric coefficient which is 1 and negative if you want here and then that is equal to + being formed rate of formation of B / the stoichiometric coefficient which is 2. So here one particular aspect that we needs to be looked at is the symbol so here I guess we need to put in your understanding so if I am calling already loss of A I guess better it is not to have a native term here if I am not talking about loss here then I could have the negative term if I am already talking about loss here.

So it is always better to look at the magnitude we will see why I guess that is obvious because when we have in our mass equation we already have rate of formation – rate of loss. Say if you again write rate of loss equal to the negative of something right this is going to end up being positive here the second term here so that is what we do not have so just right rate of formation – rate of loss and we will just write the magnitude of the rate of loss which is what we have in this case to be K CA right.

So that is what we have here the rate of loss of your particular compound A is KCA right and that is something we just looked at yes and obviously this is source equation where we looked at yes because identified it as loss and having a positive here if I did not I will have the negative symbol their right so let us see what we are up to next I guess.

So we are obviously going to apply this on batch reactor their and it is for the mass balance on compound A and then you know the system boundaries right so mass balance is as we know D CA / DT to be = rate of formation of A – the rate of loss of here this is what derive for our basic batch reactor a couple of sessions above the last session I believe last theory session I believe right.

So what do we do we are going to plug in the relevant to equations here and as we can see we have the rate of loss of A here but is A being formed in a manner now so the rate of formation of A is going to be 0. So again DCA / DT is going to be equal to 0 – and here we have K into concentration of A that is equal to - K into concentration of A so you solve that right first order homogenous differential equation.

So you end up with CA = CA naught into E power – KT right I believe obviously this is similar to what we solve for when we looked at A goes to B 2 right that does not come up in picture here not yet anyway and we will see why so anywhere here we have the concentration of A right but obviously let us say some one going to ask you why do I calculate the concentration of D2 right.

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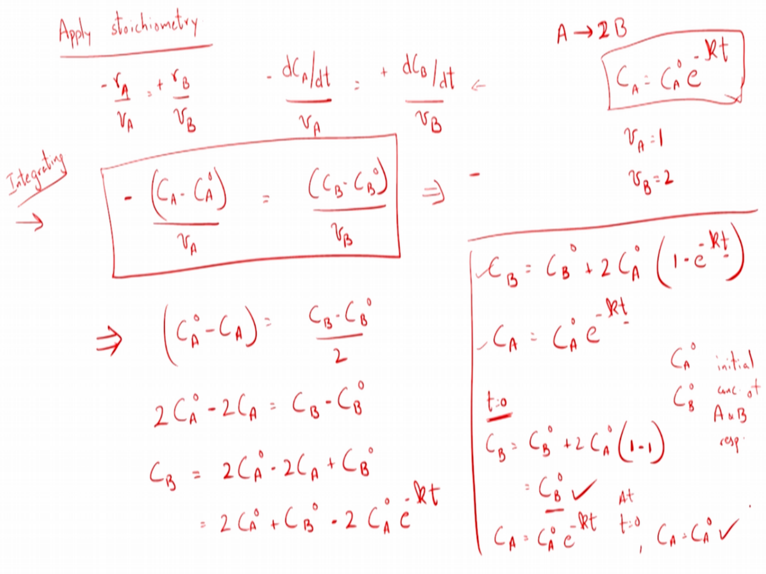

Apply stoichiometry

$-\frac{r_A}{\nu_A} = +\frac{r_B}{\nu_B}$

$-\frac{dC_A/dt}{\nu_A} = +\frac{dC_B/dt}{\nu_B} \leftarrow$

$A \rightarrow 2B$

$\boxed{C_A = C_A^0 e^{-kt}}$

$\nu_A = 1$

$\nu_B = 2$

Integrating $\rightarrow$

$\boxed{-\frac{(C_A - C_A^0)}{\nu_A} = \frac{(C_B - C_B^0)}{\nu_B}} \Rightarrow -$

$\Rightarrow (C_A^0 - C_A) = \frac{C_B - C_B^0}{2}$

$2C_A^0 - 2C_A = C_B - C_B^0$

$C_B = 2C_A^0 - 2C_A + C_B^0$

$= 2C_A^0 + C_B^0 - 2C_A^0 e^{-kt}$

✓ $C_B = C_B^0 + 2C_A^0(1 - e^{-kt})$

✓ $C_A = C_A^0 e^{-kt}$

C_A^0, C_B^0 initial conc. of A & B resp.

t = 0

$C_B = C_B^0 + 2C_A^0(1-1)$

$= C_B^0$ ✓

$C_A = C_A^0 e^{-kt}$ At t = 0, $C_A = C_A^0$ ✓

So they are different ways but in easier way would been to look at the stoichiometric so we are going to look at applying stoichiometric right and I guess in this case we talked about this earlier right rate of particular compound of A stoichiometric of A = rate of loss of formation of B / stoichiometric coefficient of B and in this case while A is being lost B is being formed.

So this is what we have with respect to the stoichiometric here right so we are going to substitute with the material balance so more or less what is this mean – DCA / DT that I rate I guess right by stoichiometric coefficient of A will be equal to + DCB / DT / stoichiometric coefficient of B so in this case what do we have the equation we have is A goes to 2B right we have A goes to 2B so let us plug them here so that is going to be and again C differential right so what is that going to be C2 – C 1 as not CA – CA naught / stoichiometric coefficient of A right we are taking about with respect to time obviously.

And so again the change here the change here and that is going to be = what is this place here CB – CB naught here / stoichiometric coefficient of B so this is obviously after integration right the change in after this comes about after integrating the previous equation right and this is what you see here right CB / CB naught I guess so let us plug in the relevant values and here we are going to have so this is particular what do we say equation you are going use throughout the class so thing what remembering where we have that from so more or less – RA / VA = RB / VB Mu B and more or less rate is DCA / DT RC is DC / DT.

So and then integrating particular equations here integrating this equation here and then plugging in the relevant values we end up with these particular sets of values right or these set of equation is so now let us plug in what we have here so far I guess we know that CA = what now I think we have CA = CA naught into E power = KT right that is what we have here in previous equation is and we also know that the stoichiometric coefficient of A is 1 and stoichiometric coefficient of B = 2.

So if I plug those values in here what is that I am going to end up with here I guess I am going to have CA naught – CA substitute at that I guess = CB – CB naught by 2 right let us see if we made any issue any issue with the symbols no think we are on the right track right. So let us solve for B and then plug for CL later on so CB or thus would be two times of CA naught – 2 times of CA will be equal to CB – CB naught right and that would mean CB = 2 times of CA naught – two times of CA + CB naught right.

So that would then mean two times of CA naught + CB naught right – two times of what do we have here we know that CA= CA naught into E power – KT so plugging that here CA naught into E power – KT right so this is what we have so I am going to continue working it out here and let us further it I guess so we have CB = CB naught + 2 times of CA naught into what else do we have here 1 – E power – KT right.

So now that and what was the CA equation I guess CA = CA naught into E power – KT so I believe we are on the right track there and we are done with that. So what are CA naught and CB naught of obviously hey are the initial concentration initial concentrations of A and B respectively right and with this we can now solve for A B at any given time T right that is what you see here right is and thus obviously we are going to go through that in detail.

So if you want to you can plug in time = 0 and time = infinity and check your particular equations so let us time = 0 so let us see what CB transform to it will be CB naught + 2 times CA naught into 1 – E to the power of 0 this is 1 1 – 1 so that is equal to CB naught so that is I check right at time equal to 0 CB = CB naught that is something that we know let us say solution for our answer not solution I guess the check.

And similarly here again if I plug it in a CA = CA naught into E power – KT right if I plug in time = 0 right what will that be C again CA = CA naught and that again is the check here right so again if we plug in infinity what would infinity would it be if it going to be at equilibrium let us say I think we are going to look at right. So if A is going to B or 2B you would expect that all of is going to be consumed and hopefully that is what we are going to see here.

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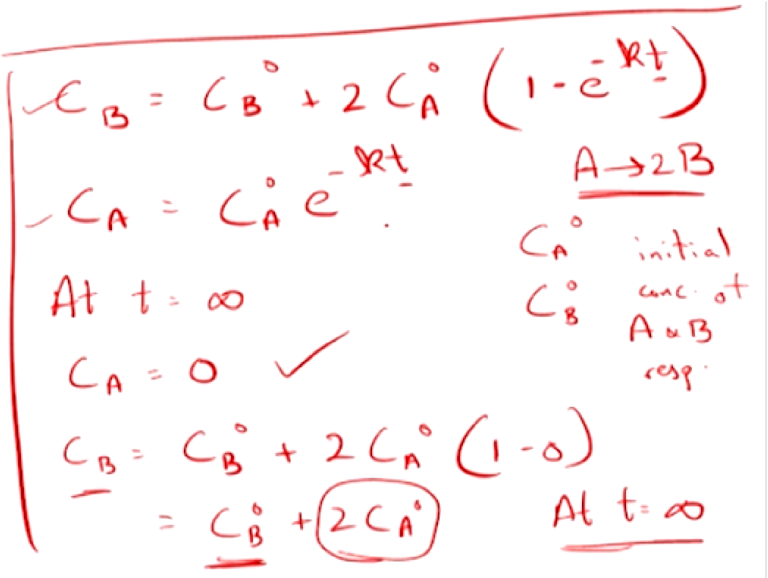

$$C_B = C_B^0 + 2C_A^0\left(1 - e^{-kt}\right)$$

$$C_A = C_A^0 e^{-kt}$$

$A \rightarrow 2B$

C_A^0, C_B^0 initial conc. of A & B resp.

At $t = \infty$

$C_A = 0$ ✓

$$C_B = C_B^0 + 2C_A^0(1 - 0)$$

$$= C_B^0 + \boxed{2C_A^0}$$

At $t = \infty$

So at time T = infinity right and that is what you see here and plug in T = infinity you see CA = 0 is that is what you expect and CB will be = CB naught + 2 time CA naught into 1 – 0 that is equal to CB naught + 2 times CA naught so this again is that time = infinity so what is that mean so at equilibrium I guess you will have what is that pardon me here all the initial CB naught present and also twice the concentration of A present why is that because we know that each mole of A we are forming two moles of B right.

So that I what we see here so the check with respect to the time = 0 and time = infinity is done and this is with respect to batch here.

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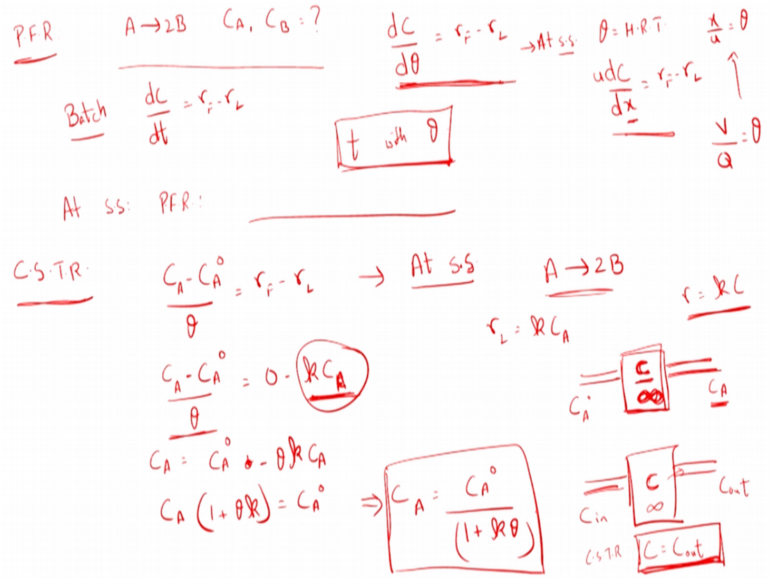

So next we will move on with respect to the derivation for the plug flow reactor right and what is basic reaction here again we are still talking about A goes to 2B and we are trying to solve of concentration of A and concentration of B and what are they I guess right so plug flow what are the basic equation here and I believe it is DC / D theta = rate of formation – rate of loss and again rate of theta what is that mean?

Theta is hydraulic retention time right and what was this equation from or where did we get this from U DC / DX = rate of formation – rate of loss so what is this mean again concentration is changing with distance and not with time that something you need to keep in mind so obviously X / U right we are saying that hydraulic retention time or more or less V / Q is theta and that is where we end up with X / U = theta here right and that is how we have here right.

So we have DC / D theta = rate of formation – rate of loss of compound and you have this particular set up and so on so. So I guess we can work everything out but as we see the only difference between the batch reactor equation DC / DT = rate of formation – rate of loss this is for the catch reactor right and one for the plug flow is that you just replace T with theta right and this obviously is at steady state that is one think you obviously need to keep in mind.

So at steady state so solution for your plug flow reactor for the above scenario what is that going to be the same going to be the same as the previous case but we just need to replace T with theta right. So and that we will done with the plug flow reactor and let us move on to the continuously stir tank reactor I guess right CSTR now and the first aspect is going to be again mass balance and what is the basic mass balance I believe it was CA – CA naught whole by theta = rate of formation – rate of loss again now differential equation here again this is the equation for the CSTR at what is this please at steady state obviously this is at steady state.

So let us go on with looking at what we have here again we have A goes to 2B right so if I am applying it on this particular case so CA or lets us switch them around to guess is A / CA – CA naught by theta = A being formed in any manner no that is going to be 0 – K rate of loss is again what now K into concentration of A that is what we have here and – KC A right and that is what we have here and say again we can end up solving for CA = what we say CA naught right + not + I guess – theta into KCA is that right.

Let us look at if our calculation for one second here please okay so I believe I can understand what the issue here is. So here we have KCA term here right I to need to bring that over to the left obviously right anyway CA = CA naught – theta into KCA if I bring this term over here CA into 1 + theta into K = CA naught right and then what next please and then it is going to be CA = CA naught by 1 + K theta right.

So this is with respect to your CSTR so the key here is weight have missed it the issue here is that you know term here is input coming in Q in or C in right and here is CA naught and here we are defining in and out CA naught and CA right and this is what we have. So for a CSTR right and this is the key here and that is how we end up with rate so we want to know the rate of this particular loss of compound of A here and this we say = C the concentration of compound of A inside the reactor is C and that we know is KC rate of loss of the compound but where we saying = KCA now.

So the key is that because this is continuous stir whatever the concentration is inside the reactor will be the same as the concentration leaving the reactor right. So that what is that mean now so if you have C in and you have C out right and this is C what is this mean C and C out are going to be the same right make sense hopefully because this is a continuous stir reactor. So whatever is coming in it is going to be instantaneously diluted and then you have the relevant equations and then it is going to flow out right.

So obviously in CSTR the key is that the concentration inside the reactor and the concentration outside the reactor are the same so that is the reason why when we are writing the rate of loss of this particular compound we directly write this as concentration of A that is leaving the system or even within the system would which is going to be the same right so that is the aspect here so where we here so CA = CA naught / 1 + K theta.

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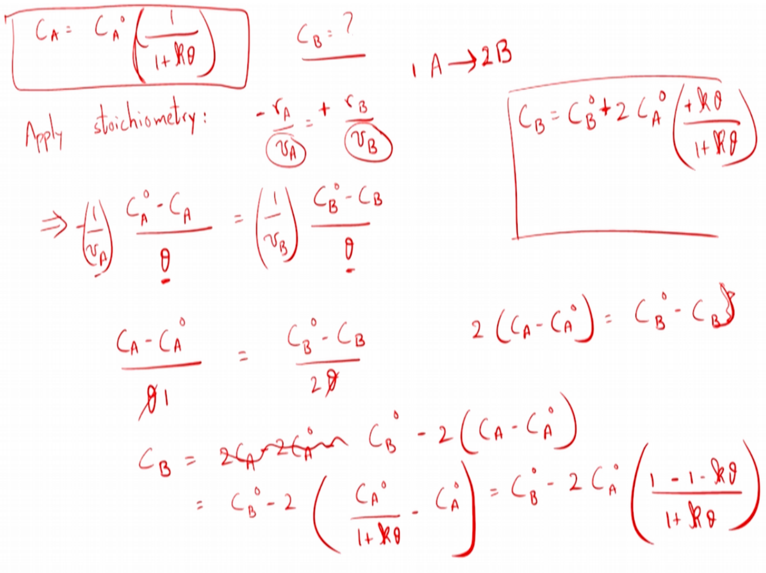

$$\boxed{C_A = C_A^0\left(\frac{1}{1+k\theta}\right)}$$

$$C_B = ?$$

$$1A \to 2B$$

Apply stoichiometry: $\frac{-r_A}{\nu_A} = \frac{+r_B}{\nu_B}$

$$\Rightarrow -\left(\frac{1}{\nu_A}\right)\frac{C_A^0 - C_A}{\theta} = \left(\frac{1}{\nu_B}\right)\frac{C_B^0 - C_B}{\theta}$$

$$\frac{C_A - C_A^0}{\cancel{\theta}\,1} = \frac{C_B^0 - C_B}{2\cancel{\theta}}$$

$$2(C_A - C_A^0) = C_B^0 - C_B$$

$$C_B = \cancel{2C_A - 2C_A^0}\; C_B^0 - 2(C_A - C_A^0)$$

$$= C_B^0 - 2\left(\frac{C_A^0}{1+k\theta} - C_A^0\right) = C_B^0 - 2C_A^0\left(\frac{1-1-k\theta}{1+k\theta}\right)$$

$$\boxed{C_B = C_B^0 + 2C_A^0\left(\frac{+k\theta}{1+k\theta}\right)}$$

So let us have this and again let me write that down C CA = CA naught / 1 + K time theta so this is what we have. So now again we need to have find out what concentration of B is right so same case as earlier we are going to apply the stoichiometric apply stoichiometric again the stoichiometric equations is A goes to 2 B right and for this let us see what we are going to have and so again we know that right of A or stoichiometric coefficient of A is going to – here and + here is being lost B or stoichiometric coefficient of B this is what we looked it earlier.

And so from this you know that we have the relevant equation after integrating and so on what is that we have we have CA naught – CA right but here instead of time it is going to be obviously theta right theta into what is going to be here CB naught – CB / theta and obviously here you are going to have the same stoichiometric coefficient here 1 / Mu A – 1 / Mu A and here I am going to have 1 / Mu B right so it is not time anymore this is hydraulic retention time here right so that is the key here.

So once you have this and let us plug in the relevant value coefficient A is just 1 here so 1 or theta here that is going to be = CB naught – CB / 2 theta. Theta obviously cancel out right one times this is what we have so again what do we have here please we have CB = 2 times concentration of A – 2 times concentration of A naught or the initial value – or we are going to have – value here one second please I guess let me simplify that for myself.

2 times of CA – CA naught right is going to be = CB naught – CB so if I take this whole term here to the left and side CB = CB naught – two times CA – CA naught and let us see what we have here. So CB naught – 2 times CA we know is and from here this equation here right what is CA here please CA naught / 1 + K theta – again CA naught right.

So that is going to be equal to CB naught – 2 times of CA naught and take 1 take this out I guess 1 – of 1 – K theta / 1 + K theta and that is going to be equal to going to finish that up out here and what am I going to have here i guess I am going to have CB = CB naught – 2 times the concentration of A naught and 1 – 1 so – K theta / 1 + K theta right an if I take this make this positive this is going to be a positive term view and this is what we are going to end up with right.

So let us try to wrap up the session here for today so what have been looking at for today's class we have been trying to apply what do we say? the case with respect to a reversible half reaction or irreversible pardon me.

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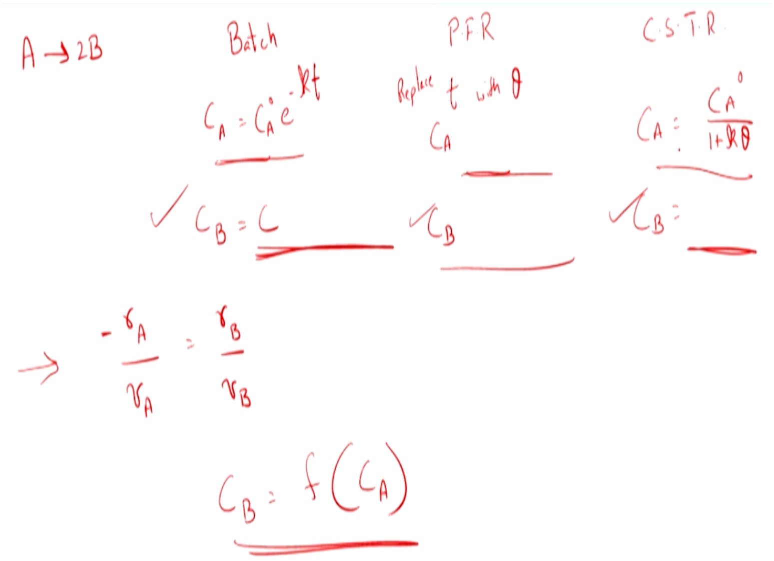

$A \rightarrow 2B$

Batch

PFR

C.S.T.R

$C_A = C_A^0 e^{-kt}$

Replace t with θ

C_A

$C_A = \frac{C_A^0}{1+k\theta}$

✓ $C_B = C$

✓ C_B

✓ $C_B =$

→ $\frac{-r_A}{\nu_A} = \frac{r_B}{\nu_B}$

$C_B = f(C_A)$

So we have been looking at A goes to 2 B right and we looked at applying them for the batch for the plug flow and for the CSTR right so batch reactor I guess first do come up with mass balance on A we end up with CA or = CA naught into E power – KT pardon me and the same case is that and I believe we end up calculating CB to be some value which I am unable to recollect let us see if I have that here on my set of slides here CB = where do we have here and here we have 2 CA naught + CB naught.

Anyway we have the relevant equation their right and for the plug flow through what do we do here we only change T or replace T with theta and we end up getting C values and CA values here right same case here and CSTR are two different case we work them out CA and CB let us see what is this that I have here CA = CA naught by 1 + K theta and again we end up with the relevant equation here.

So did we end up with CB though CA from the mass balance right CB how did we get that is from your stoichiometric again rate of A stoichiometric coefficient of A = RB / stoichiometric coefficient of B and because A is being lost we have that as negative and then I guess for batch we said it is DC / DT for plug flow DC / D theta.

And again so hence forth with CSTR and we were able to relate the concentration you know we are going to express it as concentration of function of concentration of A right and that is what we were able to do here with this particular equation and then we calculate the concentration of

B for all the three cases right. So with that I guess I will wrap up for this session and we will continue the relevant aspect or one another reversible reaction case in the next session please thank you.