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

## Module No # 02
## Lecture No # 10
## Rate of Reaction – II
## Mass Balance on different types of Reactors

Hello everyone so we are back here again so we have been discussing I guess kinetics right and in that context I am going to model different system or natural system engineered as in your activity sludge process right or your flash mixture for that matter or any other unit process right or you can also look at how what do we say concentration of various compounds change of distance of time in distance with your natural systems right that is what people are concerned with about.

So for that we looked at the consent of defining systems as various reactors so right we looked at batch reactors continuously stir tank reactors and plug flow reactors right and we also looked at defining the concept of mass balance. So that is what we looked at in previous session so today we are going to look how to apply the mass balance to these three sets of reactors right.

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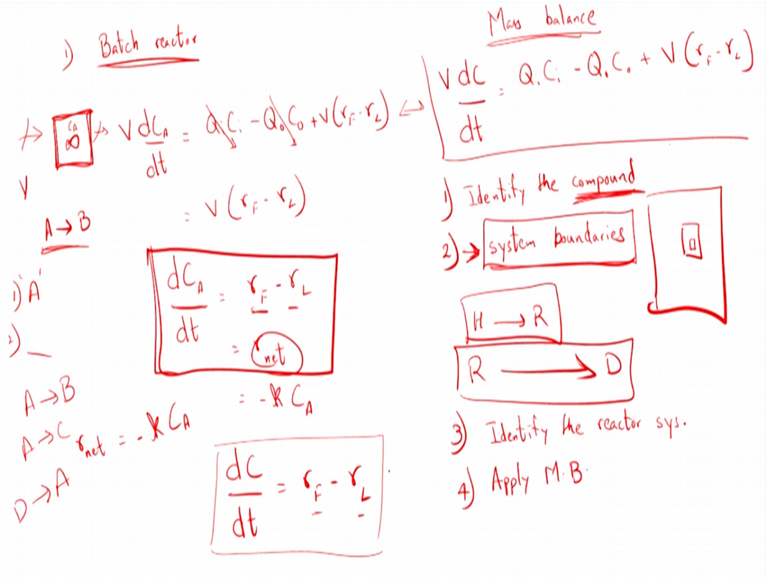

So let us go through I guess so what did we look at last time a batch reactors so that is what we are going to start discussing today and the mass balance concept mass balance and equation that we typically end up using V DC / DT = QN CN – Q out C out + volume into rate of formation and – rate of laws.

So when are you applying the mass balance 3 aspects that you need to look at I guess let us see what they are couple of aspects at least so first identify the material or compound identify the compound but you are trying to conduct the mass balance upon right this is the first aspect now always look at that and the second major aspect is identify the system boundaries.

So identify or define your system boundaries for example I am looking at whole room or am I looking at whole building or what are my system boundaries or just about let us say 1 meter from the podium so what are my boundaries or is that let us say haridware to Roorkee stretch or you know that includes or it is from Rishikesh to Delhi or what am I trying to look at right my system that I am concerned with and then I am going to try to identify the kind of ideal reactors identify the reactor system right.

And then apply mass balance say again major aspect is identify compound right you are only going to apply mass balance in particular compound and then the what do we say key lies in identifying the system boundaries or the right system boundaries. So you will choose them based on what you want and also based on what is feasible to so we will look at those later again. The first aspect we are going to apply the or the first kind of reactor going to apply the mass balance to is the batch reactor.

So we talked about what the batch reactor is it is a closed system that is obviously continuously stir or continuous mixing I guess or completely but the key is that there is no flow coming in or going out. So I am going to apply these particular mass balance equation here and what is that going to be here is V is the volume of the system here right these are the system boundaries here so let us say I am conducting the particular mass balance on a compound A which is being lost and transforming into B I guess right.

And so here I am trying to identify my compound so the first it is A compound A and the second aspect is identifying system boundaries that something that I have done say it is a beaker and the lab identify the system and then identify the reactor system so I see the obviously I know it is a batch reactor then apply the mass balance so let us apply the mass balance so VDC / DT right C is not concentration of compound of A within the reactor right.

C obviously the concentration of A within the reactant V is the volume = so now I have the terms like Q in C in – Q out C out + volume into rate of formation – rate of loss and obviously now this is a closed system as in there is no flow coming in and there is no flow going out so what is that mean the first two terms are irrelevant so that is equal to just volume into rate of flow formation – rate of loss of the compound.

So that will more or less translate into DCA or DC / DT = rate of formation – rate of loss or R net and in this case I guess with the background that we have what is R net = I guess A is being lost so that is = - K times concentration of A right and so I can now solve for the relevant equation right.

But again if you are just looking at batch reactor what is the take home message I guess this is the take home message for a batch reactor particular compound DCA / DT or DC / DT = R net so in our example we said A goes to B is the only reaction that we are looking at but obviously if there are multiple reaction let us say A going to C or D forming A and so on you will write down the relevant R net RF – RL and you will get the relevant equation.

So again what is the take home message here for a mass balance for your batch reactor DC / DT = rate of formation of the relevant compound – rate of loss of that particular compound right. So people makes on petty mistakes in these cases when they calculate rate of formation laws but keep in mind that the rates always depend upon your reactants right so that is the key here so now we have done with batch reactor let us move on to the plug flow reactor right.

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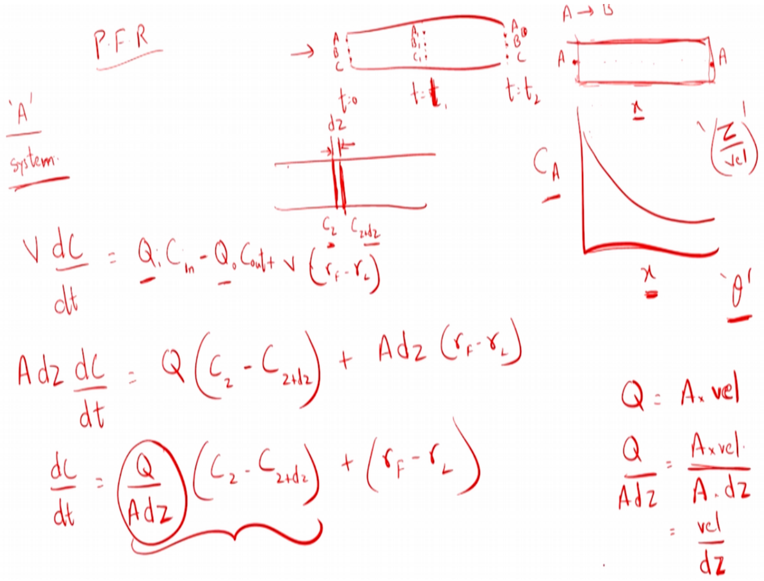

So plug flow reactor right that is flow system right so the atoms or molecules come through at the same point of time they also exit in same point of time right for example A and B and C are here at particular point time 0 so after time tax let us say or time T1 pardon me they will still being at same lateral position A, B, C and they will also exit at the same time A, B and C at time = T2 right so there is no longitudinal mixing here I guess right.

So anyway plug flow reactor as we talked about usually what do we say unit systems I guess and also reverse canals and so on. So let us look at applying this mass balance equation here so what is this now we are let us say trying to look at compound A that is has relevant reactions and then we need to identity the system boundaries so system boundaries and what is the issue here though the issue here is that compound A let us say is coming in here and there are various reactions taking place right and by time here again by compound comes here it is going to be lesser concentration.

So let us say A is decaying to B right so A is being lost during the course of this particular travel from point this point to this point here right. So what is happening to concentration let us say deceasing let us say you know yes this what I have but here if it is concentration of the Y axis what is it changing with changing with X up so it is not changing with time changing with distance right so the this one fundamental mistake most people make this.

So as it travel down the or along the course of reactor A the concentration of A changes with distance right. So people I guess say time it is not time just you can call it look at it by talking about hydraulic potential time we are going to talk about what it is later so keep in mind that in plug flow reactor your particular variables change with distance and not with time so for that something that need to keep in mind I guess and we will see what it is about.

So here now as it is I change with time with distance pardon me so I cannot apply the mass balance over the entire system here right so what do I need to do so there are two ways to go about it so we will look at both the aspects so one is to choose a thin film within which a concentration is constant right but the concentration at this phase is CZ let us say and the concentration of the outlet is what shall I say CZ + DZ okay and the thickness of this particular film is DZ.

Concentration of the inlet of this phase is CZ C subscribe Z and concentration of outlet phase are phase CZ + PZ right and the thickness of this film is going to be DZ and what was out initial mass balance equation please V DC / DT = QN CN – Q out C out + Z volume into rate of formation – rate of loss right this is what we have. So assuming that the flow it does not change obviously that is the case here right and what is the V here the cross sectional area of that particular what do we say film or this cross section area right.

A into DZ is my volume here right and DC by DT right = Q times the Q is constant Q in = Q out what is at inlet it is CZ CI – C inlet right = CZ – what is it at the outlet – CZ + DC right + volume again is A DZ into rate of formation – rate of loss right so what do I have here again I divide here by AD D I guess right. So DC by DT = Q by A DZ right let us say that I what I have here and what else do I have here CZ – CZ + DZ right + rate of formation – rate of loss right.

So this is what we have here right at steady state we have the relevant what do we say transformation. So first we are trying to go into try to look at what this is right and flow what is flow I guess Q = cross sectional area into velocity yes hopefully that says yes cross sectional area into velocity so how can I transform this particular set of variables Q / ADZ = 1 what now area into velocity right again cross sectional area into DZ right so this is going to be velocity by DZ right.

So what is distance by velocity what will that give you an idea about that is going to be time and this in case it is going to be hydraulic retention time I guess right. So that is going to be = 1 / D theta right so I guess I will do this over in the next page so what did we have here.

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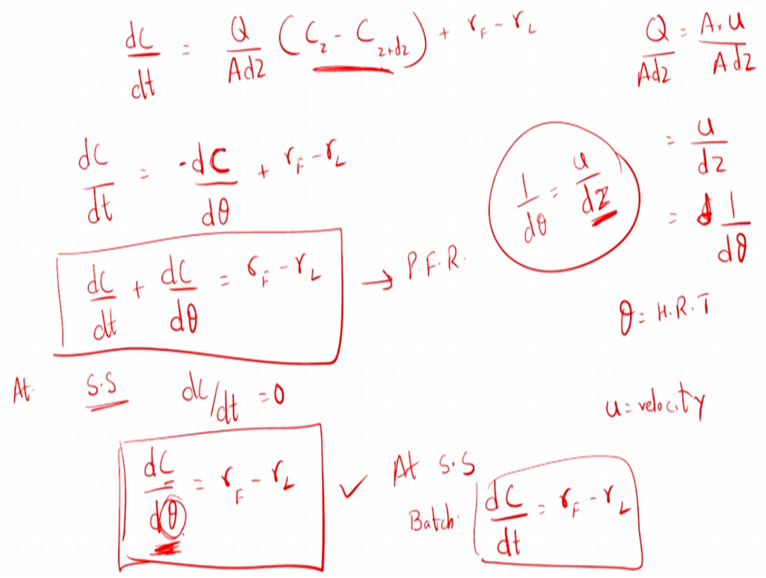

$$\frac{dC}{dt} = \frac{Q}{A\,dz}\left(C_z - \underline{C_{z+dz}}\right) + r_F - r_L \qquad \frac{Q}{A\,dz} = \frac{A \cdot u}{A\,dz} = \frac{u}{dz} = \frac{d1}{d\theta}$$

$$\frac{dC}{dt} = \frac{-dC}{d\theta} + r_F - r_L \qquad \boxed{\frac{1}{d\theta} = \frac{u}{dz}}$$

$$\boxed{\frac{dC}{dt} + \frac{dC}{d\theta} = r_F - r_L} \rightarrow \text{P.F.R.}$$

$\theta$: H.R.T

At $\underline{\text{S.S}}$ $dC/dt = 0$

$u$: velocity

$$\boxed{\frac{dC}{d\theta} = r_F - r_L} \checkmark \quad \text{At S.S Batch: } \boxed{\frac{dC}{dt} = r_F - r_L}$$

So DC / DT = Q / A DZ concentration at inlet – concentration at outlet + rate of formation – rate of loss right and so that we mention this Q = area into velocity by and Q / ADC = by ADZ and that is equal to U /DZ and that is equal to D1 / D theta and here we have a new term what is theta now hydraulic retention time right that is what we have here. And so this transforms to DC by DT = D and what is this here I guess – DC this is – DC by D Theta + rate of formation – rate of loss right.

And so DC / DT + DC / D theta = rate of formation – rate of loss right so this is the equation for your plug flow react right. So at steady state what is steady state I guess there is no change in a any variable with time so at steady state DC / DT will be equal to 0 so now I will end up with DC / D theta = rate of formation – rate of loss of the particular compound right so that is what I have here yes again this is the taken home message obviously at steady state right.

So if you can look at the similarities with respective what we derived for the batch reactor so this for a plug flow reactor for batch what was it now it DC / DT = rate of formation – rate of loss again so the difference here obviously is that with for the plug flow it is not DC / DT but DC / theta.

Theta is the hydraulic retention time but again what is that due and idea about how it changes with distance right because here we have 1 / D theta = U / DZ and what is Z change with distance and again keep in mind for the plug flow obviously the system variable changes with distance so that is what it means right.

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$$\frac{dc}{d\theta} = r_f - r_L$$

u: vel

$$u\frac{dc}{dz} = r_f - r_L$$

At S.S.

So are to simply that let us say DC / D theta = rate of formation – rate of loss or what is this equal to U into or the velocity into DC / DZ = rate of formation – rate of loss this is at study state obviously U is the velocity here right and this is what we have yes so this is one way to solve it from the relevant equation so this is much simpler way obviously for that we need to have some background about relevant what we say fundamental equation.

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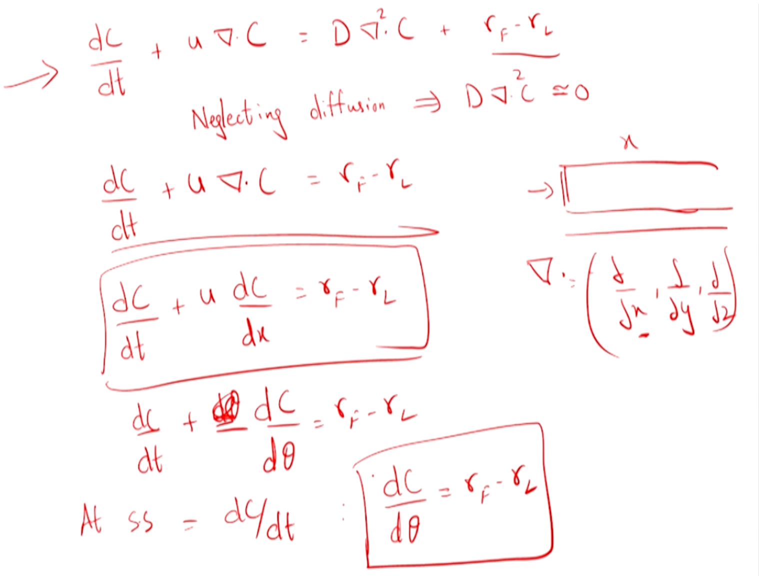

$$\frac{dC}{dt} + u\nabla\cdot C = D\nabla^2\cdot C + \underline{r_F - r_L}$$

Neglecting diffusion ⇒ $D\nabla^2\cdot C \approx 0$

$$\frac{dC}{dt} + u\nabla\cdot C = r_F - r_L$$

$$\nabla\cdot = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$$

$$\boxed{\frac{dC}{dt} + u\frac{dC}{dx} = r_F - r_L}$$

$$\frac{dC}{dt} + \frac{dC}{d\theta} = r_F - r_L$$

At ss = $dC/dt$ : $\boxed{\frac{dC}{d\theta} = r_F - r_L}$

So what was our fundamental mass balance equation if you remember I guess DC / DT + U and del C = diffusion coefficient into del square C + source are seen which is nothing but rate of formation – rate of loss this is the second way to derive what we looked neglecting diffusion here neglecting diffusion right that means D del square C = 0 right. So here what are we left with DC / DT + U del C = rate of formation – rate of loss so in a plug flow I guess right the concentration is only changing with one dimensionless I say.

So del what is del more or less del uses an idea about Dou / Dou X Dou / Dou Y and Dou / Dou Z del product but if it changing with 1 dimension what is this transform into let us say it is changing in the X direction let us say. So DC / DT + U into DC / DX = rate of formation – rate of loss and we are done with our relevant equation right so this is similar to what we have derived earlier again what is this I guess DC / DT + DC / D Theta DC / D theta = rate of formation – rate of loss.

So obviously if it is at steady state right means DT / DC = 0 and that ends up with DC / D theta = rate of formation – rate of loss so that that is what you see here right. So again if much easier you have understanding about the basic equation but you can get by with looking at the other equation to. So again this can be applicable at stead state for a any plug flow system if you have apply the if you identify the system as plug flow right so we are done with that.

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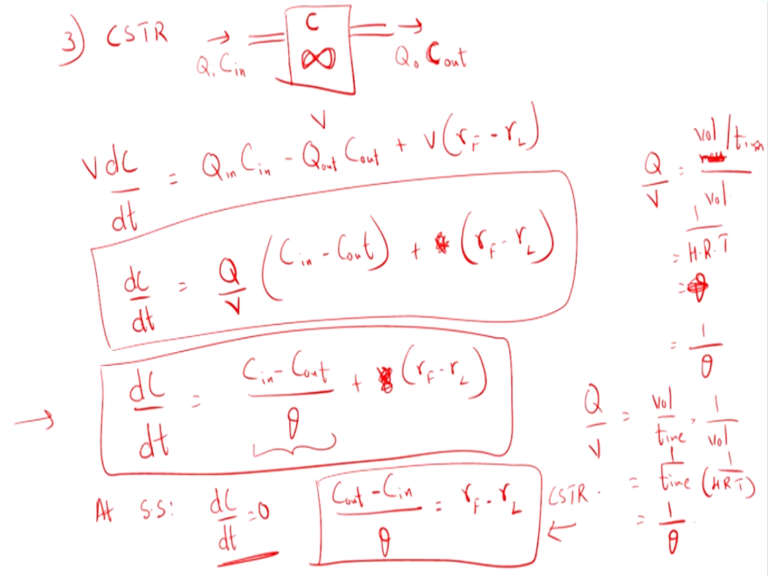

So the next aspect obviously the third kind of reactor is continuously stirred tank reactor right and what is this about we have continuous flow coming in we have continuous flow going out right and it is either always continuous stir coming out completely mixed so here is the key is that we need to identify the always either continuously stirred out completely mixed s here is the key is that identify the variables let us do them now the flow coming in flow going out volume of the reactor right.

And concentration of the compound coming in concentration of compound going out right and then what else and then concentration of compound inside the reactor so these are the variables that we are identifying and we will see why they are relatively important I guess right so now let us look at our mass balance equations so we DC/ DT = Q in C in – Q out C out + Volume into rate of formation of compound – rate of loss of the compound right.

So this is what we have is so let us try to transform this further so we can have now I guess what is this DC / DT will be equal to I am assuming Q in = is going to be equal to Q out right in this case if not you can obviously look at that = C in – C out + volume into rate of formation – rate of loss of your particular compound so right and this is what we have here right and what is Q / V Q is mass per what is it now volume per time / volume so it is more or less or hydraulic retention time it is HRT or theta right Q / V is 1 by theta pardon me.

Let me re do that I guess Q / V Q is volume per time divided by volume that is equal to time what is it HRT 1 / HRT pardon me again right that is equal to 1 by theta so what do we see here DC / DT = C in – C out / theta + volume in rate of formation – rate of loss right this is our fundamental equation so obviously at steady state at steady state what is that going to transform into now right we are going to see that DC / DT = 0 steady state means there is no change in any variable with respect to time right.

So let us see what that transform into and I take this particular term to the left hand side so C out – C in by theta = I guess are we going to have the volume term if you are going to divide by V so we are not going to have the volume term here right is going to be equal to rate of formation of the compound – rate of loss of the compound so this is what we have for a CSTR yes and let us moving on I guess let us just rewrite this.

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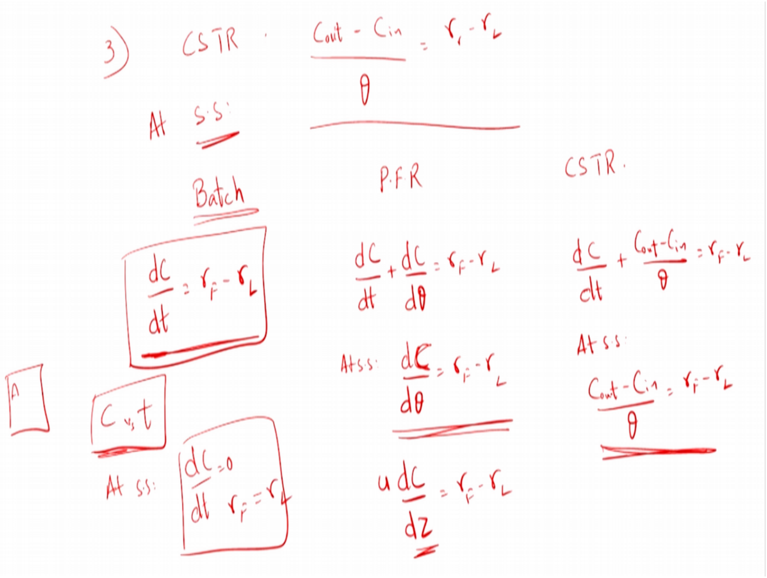

So the third case is for CSTR what did we end up with C out – C in / theta = rate of formation – rate of loss your compound I guess C out – so any way I have a take home message here this is obviously at steady state yes this is at steady state so what is the take home message here you see that the there is no differential right there is no differential equation here it is just a usual equation no differential equation here and that I guess is relatively different from what we observed with respect to batch reactant.

So let us write down what it is or what we looked at with respect to of the three cases and we have now CSTR right and so batch reactor we applied the relevant mass balance and I believe we came up with DC / DT = rate of formation – rate of loss of your particular compound for plug flow we said I believe it is going to be DC / DT + DT / D theta right = going to be = rate of formation – rate of loss so at steady state it is going to be equal to DC by D theta = rate of formation – rate of loss and for CSTR guess we said it is going to be DC / DT + C out – C in / theta = rate of formation – rate of loss.

So at steady state is going to be C out – C in / theta = rate of formation – rate of loss right so let us look at what this means. So this batch reactors obviously it is going to change with time so I have a compound here right compound A changing with time so whenever let us say someone says it is at steady state what does it mean so that means there is no more change in your particular concentration so C versus T when there is someone says there is no more at steady state that means write it has already reached equilibrium right.

So at steady state what is that transform into now DC / DT equal to 0 right what is that mean rate of formation and will be equal to rate lo loss right and you see not further change in concentration with time right and that is more or less equilibrium this is the system as reached the maximum extent possible there in your batch yet.

So in the plug for reactor the take message is that it does not change with yet as in concentration does not change with time but the hydraulic retention time or more specially with distance down the reactant now right that is what it mean keep that in mind DZ or DX whichever dimension we are looked at.

And CSTR are at steady state no differential equation right it is C out – C in / theta = rate of formation – rate of loss so without I will believe in wrap up today’s session and we are going to talk about fabrication of these particular reactor to various kind of reactors we are we will come across. So may be for now if we have enough time let us look at one example I guess right with respect to batch reactor.

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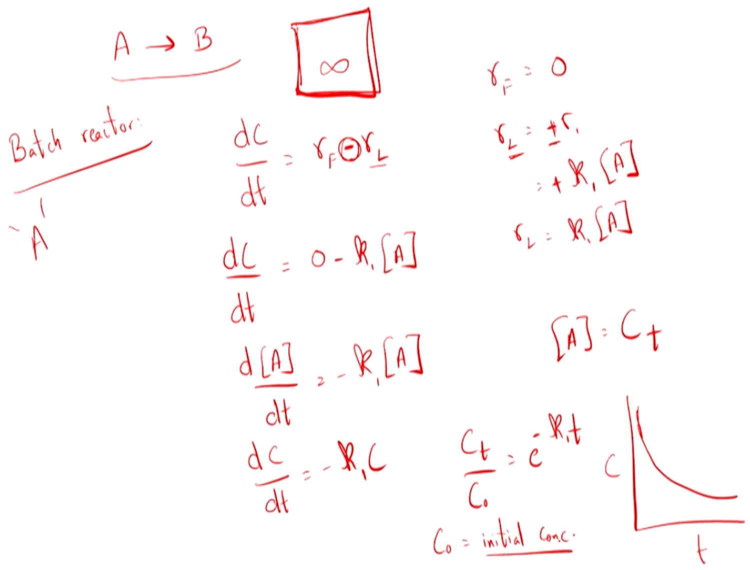

So let us say A goes to B C + A goes to B in a batch reactor and want to apply these you know to my mass balance let us say right for now let us go with simple first order equation and will be done with today once I have done with these particular case with batch reactor and what is that going to be I guess we know that it is DC / DT = rate of formation – rate of loss and here rate of formation of the compound A.

I am applying the mass balance on compound A these are my system boundaries right and it is completely mixed and rate of formation of these particular compound what is that it is = 0 it is not being formed rate of loss of the these compound is this stoichiometric coefficient which is 1 times what now anyway it is native times rate of reaction 1 and that is = - K1 rate constant rate A.

So what does DC/DT transform into it transforms into rate of formation of 0 – okay if I am already using negative here obviously do not need to use negative term here again I guess this is some need to be careful about if I am already having the sign here right indicates the right of loss is being subtracted I again I am not going to look at relevant sign here but only the magnitude here.

So rate of loss here is K1 times A it is 0 - K1 times concentration of A so DC or D concentration of change if the A with respect to time = 1 K1 concentration of A right or if it say it is CT let us say you know if I am saying A = CT so DC right so that integrates more or less CT / C naught = E power – K1 into T right CT / C naught and what is this mean right C and times exponential decay that is not a good figure but that should do now right and C naught is the initial concentration obviously right.

So I guess with that we are going to end today's session and will take this through with respect to the other reactors such plug flow and batch and then look at the bit more of your complex system I guess and that is it for now and thank you.