

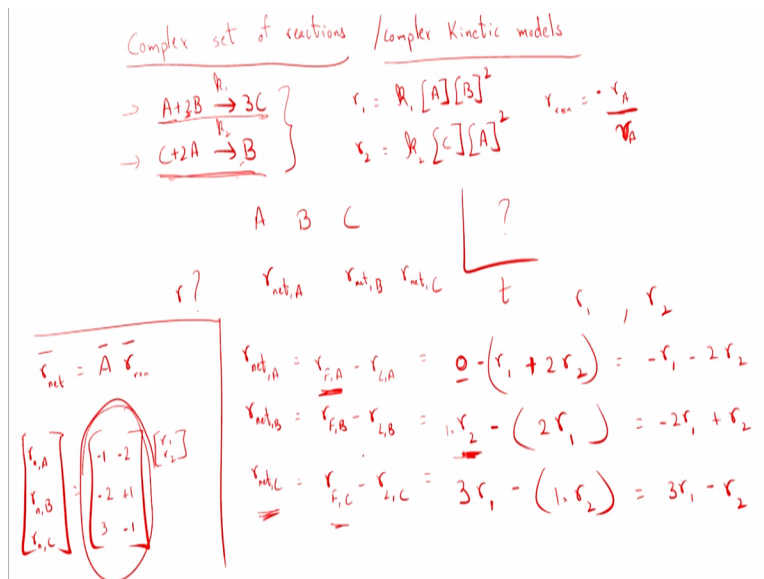
**Environment Engineering: Chemical Processes**  
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**Module No # 02**  
**Lecture No # 09**  
**Rate of Reaction – II**  
**Types of Reactors**

Hello everyone welcome back to we were discussing kinetics right and we are discussing the factors effecting the rate of reactions and the most or in general the usually encountered factor is the concentration of your reactants the key here is that is not the product is always concentration of the reactants that define or you know going to regulate the rate of your particular reaction right.

Then we also looked at temperature I believe right and then we also looked at stoichiometric is relevant your particular reaction or rate of the reaction being related to your individual rates of different compounds right and then we believe started moving on two complex sets of reaction.

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Let us see or when you have a complex kinetic model right you want to model this later on so here we started looking at or consider at set of examples obviously this is application even when you have 20, 30 or so reaction now right. So how would you go about this let us say if you say

20 such reactions now so here you have A and B what do you say reaction to form C and again I guess C and A reacting to form B and so on right how do you go about it?

So let us look at that I guess first aspect is to write down rate of reaction one and what is that I guess and what is that going to be let us say rate constant is  $K_1$  and  $K_2$ . So rate constant is 1 and 2 right let us going to be  $K_1$  times concentration of A time concentration of B raise to the power of 2 right yes and what about rate of reaction 2 that is going to be equal to  $K_2$  the rate constant and concentration of C in concentration of A raise to the power 2 so that is what we have here right.

But here let us say I am not concern with the rates of reactions I want to know how A, B and C change with respect to let us say time how do this concentration change with time now for that I need to be able to know or model the relevant rates of the reactions what is  $R_{\text{net}}$  of A,  $R_{\text{net}}$  of B, and same case  $R_{\text{net}}$  of C right. So first obviously I am going to use what do we say these three or express then in terms of rate of loss of A and obviously rate of formation of what is  $R_{\text{net}}$ ?

Obviously I guess and again same case  $R_{\text{net}}$  of B will be rate of formation of B – rate of loss of B and again  $R_{\text{net}}$  of C will be equal to rate of now formation of C – rate of loss of C. So let us see what it is we have here I guess so let us have same nomenclature here right so equal to rate of formation of A – rate of loss of A let us see how we can relate them to your relevant rates of reactions 1 and rates of reaction 2 right.

So let us look at that I guess how is A being formed it is being formed nowhere that is going to be 0 right – rate of loss how is A being lost it is being lost by both the reactions so what is that I guess. So we are going to have – rate of reaction is 1 because stoichiometric is 1 here and – 2 are 2 right hopefully that makes sense so  $R_{\text{net}}$  is – of  $R_1 + 2R_2$ .

So anyway S is not being formed it is only being lost to both the reaction and as we looked at earlier the rate of reactions = what now rate of let us say loss A by it is stoichiometric coefficient this is what we discussed in the last class and that is where we get these particular aspects right the rate of your loss of A and that is what we see here.

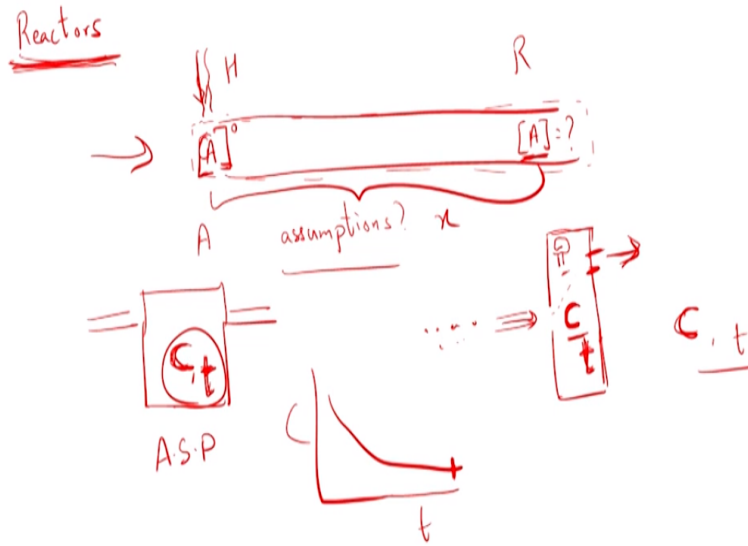
And so let us move on to B look at how these being formed B is being formed from your second reaction stoichiometric coefficient is 1 so it is going to be rate of reaction number 2 right – how is B being lost it is being lost first reaction and what is stoichiometric coefficient 2 so it is going to be 2 R2 right. And again same case pardon me not R2 it is obviously R1 again so B is being formed reaction 2 that is what we see here and guess the stoichiometric is coefficient.

So that is R2 there just add 1 in R2 and how is it being lost now it is being lost to first reaction and it is two times because it is stoichiometric coefficient is going to be 2 or is 2 pardon me and same case with R net C rate of formation of C how it is C being formed it is being formed in first reaction right and what the stoichiometric coefficient their 3 so 3R1 – how is it being lost being lost by the second reaction right and the stoichiometric coefficient is 1 so that is what we have here right.

So if we just simply here –  $R_1 - 2R_2 = -2R_1 + R_2 = 3R_1 - R_2$  right so in general what are how are we are going to express these sets of equations as. We are going to express this as matrices R net matrix is = relevant coefficient matrix relevant of the rates of the reaction matrix right so R net will be what now the matrix it as R net of A R net B and R net of C what is A going to be = I guess right you are going to have the relevant coefficients here and what are they – 1 and – 2 and what do we here I guess – 2 and + 1 and here we have 3 and – 2 right and here we are going to have your R 1 and R2 right yes.

So I believe now with this let us say you can set it up with your particular what do we say matlab or such and 1 once you can have this matrix with respect to relevant models right you can go ahead and get this done. So here we are looking at how to express that in R term in various reaction here right so that is what you see here.

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So again let us move on so the next major aspect we are going to consider is reactors right and let us first see what is relevance here and so this is going to be one of the fundamental aspects you are going to learn throughout the course of your class right. So let us take some time about understanding the relevant of the reactors to our particular case or environment engineering here right and then look at the different reactors we come across and then we are going to look at how to model them right.

So let us look at some cases now let us say there is an industrial what do we say estate near haridwar and I am Roorkee may be 30 kilometer downstream right. So let us say some industry there let us say I am going to use the site here so here we have Haridwar and here we have roorkee and let us some industry is dumping its waste right in ganga or ganga canal right let us say and the ganga canal or ganga is flowing downstream.

So I want to know let us say the concentration is  $C$  naught let us say let us say concentration of toxic compound  $A$ ,  $A$  naught and what is it at Roorkee though this is what I want to know though right so how do I go about it? So for that you know I am going to define a reactor of certain what do we say boundaries and then I am going to model  $A$  or how is  $A$  is going to change or transform within this boundary and by that what do we say once I have done with the model.

And I also consider some assumptions to make the model relatively simpler right I can end up calculating or predicting the concentration of this particular compound or toxic compound  $A$  at

Roorkee now right. So another example is let us say I am in this particular room let us say and I am looking at air pollutants let us say and someone usually burns crops let us say and let us say the wind blows here in let us say instead of door we have an door or window here right.

So the wind is coming in and going out here so an air pollutant is also transported along with the wind but let us say we have a filter or such let us say you know let us say the plant that can degrade this toxic compound this is a hypothetical case pardon me so you want to model what is the concentration of this compound in this room now right. So for that we have a relevant variables we can plug them in and then come up with how will concentration change with time here right.

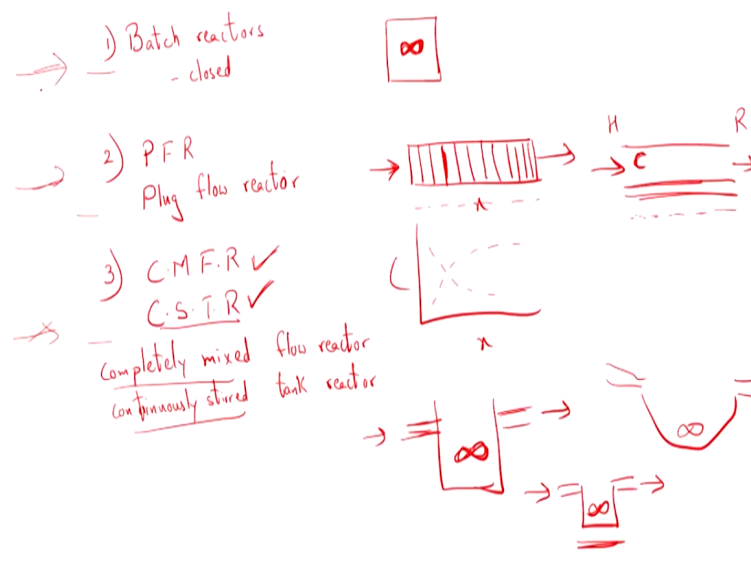
Here you are checking how is the concentration changing with distance and this particular case second or later case with respect to room let us say where the air pollutant into the door and going out through the window and may be some reactions inside the room or degrading the compound or even lead into formation of compound you are looking at how the concentration profile changes with time you can also look at how it changes with distance but that is going to be relatively more complex system right.

So anyway or even let us say you know we have your actuated sludge process here right actuated sludge process coming in and going out. So you want to know how the concentration before reaches steady state let us say or what is going to be  $X$  steady state or before it reaches steady state how is it going to change with time right and so on now. For these aspect we always need to be able to define the relevant reactors we are going to see what are the ideal case reactors.

So this is an example of actuated sludge process I want to know the concentration either at equilibrium or most basically how it changes with time in my activated sludge process right I want to be able to use the concept of reactors and then moral concentration Versus time and now I know that at equilibrium this is the concentration is going to be and this is going to my design variable right so this is what we are going to look at.

So reactors again their relevant everywhere there are three ideal case reactors let us look at what they are.

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So the first one would be a batch reactor and keep in mind these are just terms that we are assign to different scenario's let us look at what they are first case would be a batch reactor so it is a closed system right keep in mind it is a closed system no flow coming in no flow going out and such but the assumption is that it is completely mixed this is the symbol I am going to use for saying that the system is completely mixed.

The batch reactor is one that closed system and that is completely mixed right now flow coming in or going out and second phase is a plug flow reactor right similar to flow through pipe let us say right or a channel so the atoms or molecules entered here and there is now mixing here right so the concentration changes here with each distance or with distance I guess so there is now longitudinal mixing only lateral mixing right the concentration changes go along if I draw a C versus X.

X being this particular distance it can decrease it can increase and so on right so this is a case of plug flow reactor right obviously what can you what do we say use this to model so if you have canal think that we just talked about examples a Ganga canal so I have haridwar here I have Roorkee here and I have flow coming in going out and I can use the plug flow reactant model concept to look at or model how concentration of particular compound going to change between haridwar and Roorkee right.

So this is one example for Plug flow reactors application but obviously we will be having exemptions right and the third case people would come across is the completely mixed flow reactors or continuously tank reactor right so completely or completely stirred tank reactor. So we have two cases more or less the same in general what is it about now so we have flow coming in flow going out right it is a not a closed system it is a closed aspect and you have obviously it is completely mixed or continuously stirred I guess continuously stirred.

So again complete continues right so that is what this is the scenario that needs that we need to conjure up whenever someone refers to CSTR completely mixed flow reactor. So what can be approximate using this reactors let us say you can say a lake let us say lake yes but obviously there are lot more assumption involved here right especially with respect to mixing is going to have issues with respect diffusion and advection we are not going to go into detail but in the engineering what can we use that I guess.

You know any of your unit process your ASP or SPR and so on what are they more or less all of them are continuously flow coming in and going out or at least ASP pardon me we have continuous flow coming in and going out and you will in general have continuous mixing here right so you can use the concept that we are going to look into with respect to CSTR whenever you model your engineering systems.

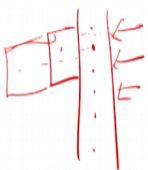
So obviously when you come across your scenario you need to be able to identify which class is it available which batch reactor plug flow reactor or a continuously stir tank reactor right and so then we can take that through. So let us move on to why or how we can model the concentration.


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Mass balance / Material balance

$$\frac{dC}{dt} + \nabla \cdot \mathbf{J} = S$$

$\nabla \cdot = \left( \frac{d}{dx}, \frac{d}{dy}, \frac{d}{dz} \right)$   
 $\mathbf{J} = \text{flux}$   
 $= \frac{\text{mass}}{\text{area} \cdot \text{time}}$   
 $S = \text{source / sinks}$   
 $\mathbf{J} : \text{Advection, Diffusion}$


net fluid motion  
Advection is transport mechanism


Diffusion - concentration  
 Higher conc. to regions of lower conc.

So for that aspect we need to talk about mass balance or material balance right and this is again a fundamental aspect here so which we are going to use whenever we are going to look at modeling various reactors or compounds with reactors right so what I guess where this from so we know that the material is conserved neither formed or destroyed right so more or less that is the case here.

So let us look at some of the applications here right so in general there is a fundamental equation here we see or change in concentration with time + the del product of flux = the source and sinks so  $\nabla \cdot$  is the dell this is the dell product right and that will give me idea about  $\frac{dC}{dt}$  or how is that particular variable change in with each of the dimensions here right whenever I say this that more or less translates into  $\frac{dC}{dx}$  of the particular flux here in this case  $\frac{dC}{dy}$  and  $\frac{dC}{dz}$ .

How this flux changing with or with each dimension their and  $\mathbf{J}$  is the flux and Flux is in case what now mass per area per time okay change in the mass of the particular compound let us say per unit area per time that is more or less flux right and then what else  $S$  is the source or sinks of that particular compound sources or sinks keep in mind that this is the fundamental equation everything else we are going to look at is they are going to derive from going to be derived from here right.



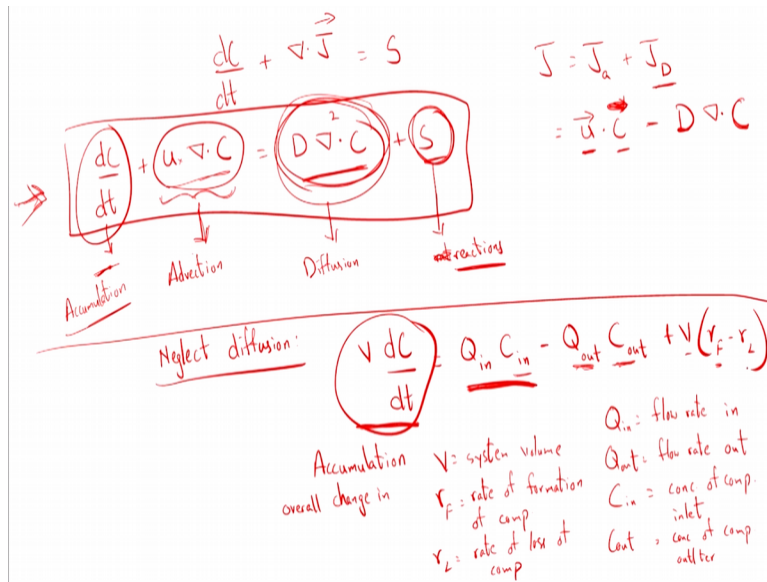
So in general in flux there are two cases one is advection the other is diffusion will not go through this in detail because this is outside the ambit of the course but it worth on understanding what it about. So for example let us say I am trying to understand advection let us say let us say you know I have a high way here right and my house is right here yes I have a dust particular here it is suspended over the road let us say and here is the wind blowing let us say wind is going to carry the dust particle to my house let us say may be 10 meters down the or (( )) (18:13) an so on.

So whenever there is a the fluid motion let us say in a direction net fluid motion right so then I can say that particular ah what do we advection can or is an important transport mechanism right important transport mechanism right so that is the case here advection I guess the other example I want to have is here let us say this is the recording class here and so here at this podium right.

And let us say there are couple of students sitting here at there are no fans running there is no fans no wind blowing it is completely sealed room now. But if open a central model I say you know if I open up a scent bottle I say so after certain amount of time the student sitting here right this is plan view obviously can sense smell this particular scent or compound why is that now because due different in concentrating radiance at the concentration radiance pardon me and due to diffusion the compound is going to transported from what do you say my podium to the student here.

And why is that because of concentration gradient and keep in mind that diffusion is random so it always flows from higher concentration to regions **of regions** of lower concentration.

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Anyway that is good enough for now we would not go into that in greater detail right we still have  $C / DT +$  the del part of flux that is the vector I guess something needs to be corrected their and so we say that the flux can be due to advection whenever there is a net flow of fluid and due to also diffusion and random and due to concentration gradient and that is = what now?

The velocity here and then obviously the concentration of particular compound + the diffusion coefficient her  $D$  is the diffusion coefficient here into del part of here concentration equilibrium and this  $I$  is going to be negative because diffusion takes from concentration higher region to lower region right so here it is negative I guess this is a negative here this is what we see here right.

So again the del part here put that on  $DC / DT$  and plug that in I guess that del assuming that the velocity is constant or does not change with dimension let us say so  $del.C = D del square C +$  source or  $sin$  so this is your final equation here so what does this so let us look at what each variable look an idea about this tells us how the concentration is changing with time the first set of variables or this  $DC/DT$  and you  $del C$  gives us how is advection affection your system right.

The transport of particular system up to your system and this particular set of variables relate to diffusion right and this respect to sources or since or you know any rates of or you know reactions reading to forming your compound or loss of your compound and so on right. So again let us look at what we have again here the first variable here  $DC/ DT$  the set of variables.

The differentials here is about give us an idea about how the concentration is changing in time or accumulation of your compound right can be negative to obviously and the second set is going to give an idea about advection let us say if there is net fluid flow how is your how is going to effect the transport of your particular compound this one is going to be diffusion and sources or sinks anyway this is outset the ambit of this course we are not going to use this in greater detail but the next equation that is derived from this is going to be the case.

So in this equation we are going to neglect diffusion okay we are going to neglect diffusion which is the case in most engineered system in environmental engineering not in natural systems keep that in mind right and so we are going to end up with  $V \frac{dC}{dt} = Q_{in} C_{in} - Q_{out} C_{out} + \text{volume into rate of formation of the compound} - \text{rate of loss of the compound}$ . So let us see what we have here so more or less if you multiply this particular equation / V and then neglect diffusion and take this advection term to right hand side this is what you end up with.

So again if you just multiply our previous equation with volume of your system right previous equation at its fundamental equation with volume of your system and take the advection term to the right and side and then neglect diffusion and then expand upon the source and sinks this is what you end up with right. So let us see what we have here what is this variable give an idea about or this set of variables I guess they give an idea about accumulation if guess.

So overall change in mass of your particular compound in that particular system boundary in respect to time right that is what you see in this particular set of variables and what is this giving you about Q in what is Q in flow rate coming in Q out flow rate of your water solution compound going out C in is the concentration of your compound at the inlet C out = concentration of your compound at the outlet right and V is your system volume RF = your rate of formation of your compound RL = rate of loss of compound right.

So again what do we have Q in is the flow rate coming in at the inlet C in is the concentration of our compound at the inlet C out is the flow rate going out of our system and C out is the concentration of the compound at the outlet V is volume of the system RF is the rate of formation of the compound and RL is the rate of loss the compound So let us see in greater detail what these are about?

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$$V \frac{dC}{dt} = Q_{in} C_{in} - Q_{out} C_{out} + V (r_f - r_L)$$

Accumulation  $\frac{vol. \times mass}{time \times vol.} = \frac{mass}{time}$   
 in  $\frac{mass}{time}$  out  $\frac{mass}{time}$  formation/loss of your comp  $\frac{mass}{time}$   
 =  $\frac{Volume \times mass}{time \times vol} = \frac{mass}{time}$   
 Batch -  $V \frac{dC}{dt} = Q_i C_i - Q_o C_o + V (r_f - r_L)$   
 PFR -  
 CSTR - ASP

So what is our fundamental mass balance equation  $V \frac{dC}{dt} - Q_{in} C_{in} - Q_{out} C_{out} +$  volume into rate of formation – rate of loss this is what we have. So let us understand what each of these set of variables set of I guess so these is the accumulation terms tight and this particular equation this Q is what do we say volume per time let us say the units and what is the concentration it is mass of your compound per volume of your what we say solvent here.

So that more or less it is equal to mass per time so that particular set of variables gives you an idea about mass coming into your system right. So what is Q and C idea giving you an idea about mass coming in or flow into your system so that is what you see here and same case Q out C out you will again be mass per time and this will give an idea about what is the mass flowing out of the system now right.

So this is the mass coming in to the system this is the mass flowing out of the system right so this is what we have and what is these terms gives us an idea about these volumes here and what is rate? Its mass per volume per time so what will that come out to be that is going to be equal to mass per time again same units as you would see their right so this will give you an idea about the formation or loss of your compound right and this obviously again what is this = to volume into concentration into mass per volume the differential is per time right that is again = mass per time.

So all the units are more or less mass per time as you see and these gives us an idea about how is the compound accumulating or you know being over all accumulation of you particular compound in the system this gives us an idea about the mass flowing in the system and this gives you an idea about how is the mass flowing out of the system or how? How much I guess and this set of variables will give you an idea about how much of it is being formed and how much of it being lost with respect to time.

So I believe we are almost out of time so quickly review what we discussed so I discussed I guess batch reactors and plug flow reactors and continuously stir tank reactors batch reactors usually used in lab plug flow again lab or engineering system or natural system like reverse CSTR either lakes or most of your ASP or most of your unit process right and for all these cases we looked at the relevant condition to describe them.

And then we looked at fundamental mass balance equation and then looked at generic equation we are going to use throughout the class it is  $V \frac{dC}{dt} = Q_{in} C_{in} - Q_{out} C_{out} + \text{volume} \times (\text{rate of formation} - \text{rate of law})$  so is compound changing with time in your system it depends upon concentration the mass coming into the system mass going out of the system and how is it either being formed or loss due to various reaction.

So in next class we are going to apply this mass balance to each of these three reactors here or reactor system I guess and I guess with that I will end the class for this session and thank you.