Water and Waste Water Treatment
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Lecture - 06
Mass Balance: Batch Reactor, CSTR and Plug Flow Reactors

Hello everyone, welcome back to the latest lecture session. Very quick recap of what we have been up to, we introduced ourselves to the concept of mass balance and why do we need to look at mass balance because if you want to understand the flow that has to be maintained in your particular reactor or your wastewater treatment plant or if the given flow. The concentration of the compound or the waste that is coming into your wastewater treatment plant.

The concentration that has to be in the effluent of the wastewater treatment plant. You can design the relevant parameters of your plant accordingly as in volume, concentration of the microorganisms, let us see. In that context, we looked at the fundamental mass balance equation.

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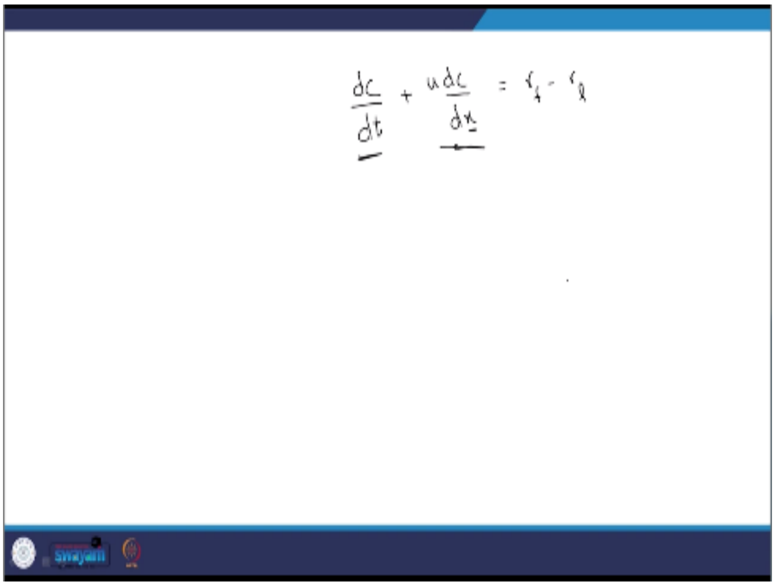

$$\underline{\frac{dc}{dt}} + u\underline{\frac{dc}{dx}} = r_f - r_l$$

$$\boxed{\frac{dC}{dt} + u\frac{dC}{dx} = r_f - r_l}$$

We see that we neglected diffusion and dispersion. The accumulation term plus u dc by dx which is due to advection, concentration change with distance. Why is this due to advection, is going to be equal to rate of formation minus rate of loss of the particular compound. This is the fundamental mass balance equation, neglecting diffusion and dispersion.

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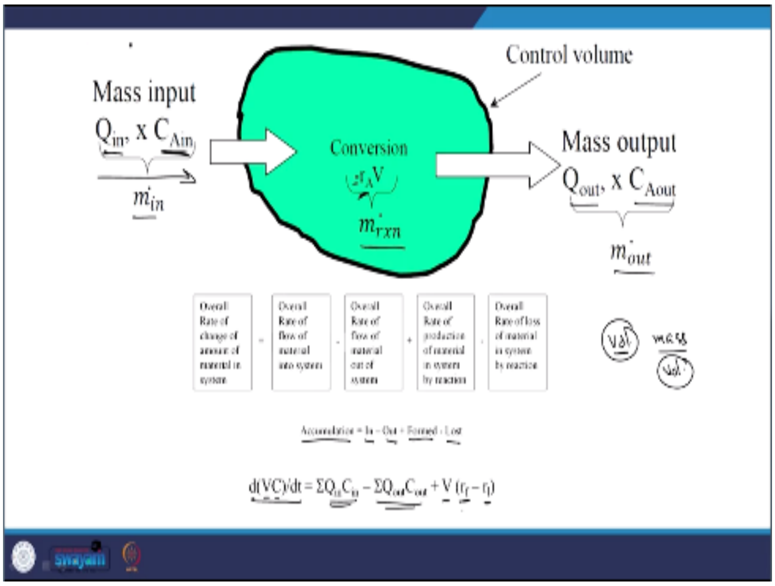

Overall Rate of change of amount of material in system = Overall Rate of flow of material into system - Overall Rate of flow of material out of system + Overall Rate of production of material in system by reaction - Overall Rate of loss of material in system by reaction

Accumulation = In - Out + Formed - Lost

$$d(VC)/dt = \Sigma Q_{in} C_{in} - \Sigma Q_{out} C_{out} + V\,(r_f - r_l)$$

We will look at understanding or try to understand the mass balance in the usual way too. We looked at the fundamental mass balance equation. Here we have the control volume. What do we have looks like if this is my wastewater treatment plants reactor, I have mass coming in due to flow Q in and the concentration of the compound in that input flow. Similarly, flow out and the compound going out along with that flow.

Mass coming in and mass going out, and also looks like the compound is being converted due to reaction. That is due to this particular reaction here rate of that particular loss of that compound. Why am I saying loss? Because we have a negative out here. To put it in the general terms, so, we have accumulation, we have mass coming in, mass going out. We have the compound being formed into reaction; compound being lost due to the reaction.

If I put this in terms of the variables that I am going to use, so, I have d V C by dt. V into C is nothing but mass as in V is volume. Concentration is mass per volume. So, if these two will cancel out, I am left with mass. It is nothing but change in mass per time within that control volume. Summation of all the mass coming in via the flow or due to advection here.

Q in C in that is something that we looked at and all the flow that is leading to loss of the mass or mass output. Mass in and mass out and then the compound being formed or lost, and we multiply by volume. That the unit stay the same here. That is what we have out here.

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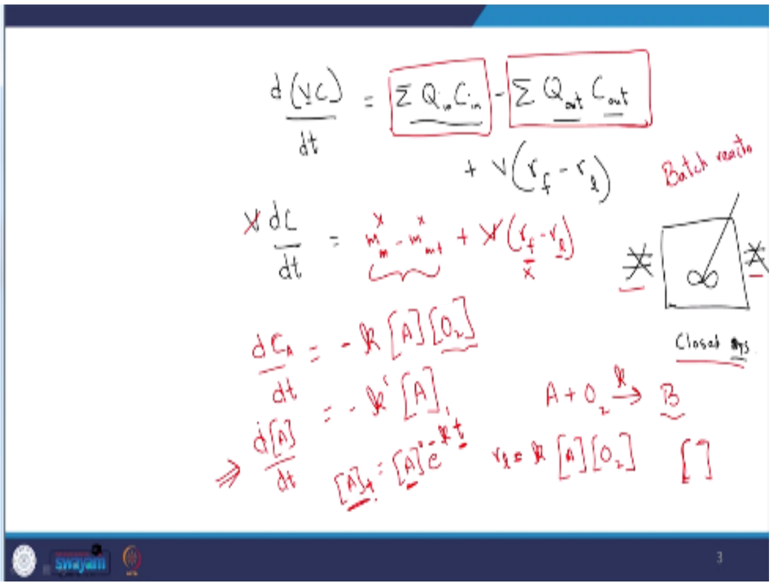

$$\frac{d(VC)}{dt} = \boxed{\sum Q_{in} C_{in}} - \boxed{\sum Q_{out} C_{out}} + V(r_f - r_l)$$

$$\cancel{V}\frac{dC}{dt} = \underbrace{\dot{m}_{in} - \dot{m}_{out}}_{} + \cancel{V}(r_f - r_l)$$

$$\frac{dC_A}{dt} = -k[A][O_2]$$

$$= -k'[A]$$

$$\Rightarrow \frac{d[A]}{dt} \qquad [A]_t = [A]_0 e^{-kt}$$

$$A + O_2 \xrightarrow{k} B \qquad r_l = k[A][O_2] \qquad [\;]$$

$$[A]_t = [A]e^{-kt}$$

Let us see what how I can transform that particular equation, what do we have? We had d V C by dt, change in mass per time within that control volume is equal to the summation of Q in and C in or mass coming in minus mass leaving via this advection or leaving the relevant reactor, need not say advection out here, Q out into C out plus volume into rate of formation of the compound minus rate of loss of the compound.

First, this term, typically, the volume of here, reactor is constant., V does not change with time dc by dt is equal to all these terms. We can transform this according to the type of reactor that we have. For example, this room now is closed, the door is closed, all the windows are closed.

If I release some compound here, now at time is equal to 0 and want to observe the changes in this particular reactor at different times, reactor is my room. To get the same concentration throughout the reactor, I keep the fans turned on. That means that I am having something like this which is a closed system, a closed system, closed system, and then it is continuously mixed.

That the concentration within the particular reactor is assumed to be constant. But note that because there is no flow coming in or no flow going out, what is it now? We do not have this mass term, this mass term is not going to be applicable in this particular example, we are talking about the room out here. There is no mass coming in mass in minus mass out is 0.

We have the equal to plus V into rate of formation minus rate of loss of the compound. The example I was trying to give is, I opened up this bottle and I released a particular toxin or hazardous chemical into this room and I left the fans turned on. The person outside the room wants to know, after how many minutes or hours, is it safe to come into this particular room?

Assuming that the compound will react with, oxygen in the atmosphere and, be transformed into harmless byproducts. There is no formation of the compound, there is only one time release, we do not need to look at that, because there is no mass coming extraneously from the system, no mass leaving the system., that is something we already looked at out here.

The compound is not being formed, it is only being lost, compound A is reacting with oxygen and is going to some other byproducts. How do I get the rate of this particular reaction here? Rate of loss is equal to the rate constant of this reaction k times the concentration of the reactants always which are this., that is what we have out here.

V dc by dt cancel out, this V and V dc by dt is equal to rate of formation is 0, that A is not being formed here, is equal to minus rate constant of this reaction times A times O_2. If I know the concentration of O_2 in this particular room and if I assume that it is more or less constant, I can say that it is equal to minus k dash concentration of A. This is C, this C itself is concentration of A, so, I can write it as d.

These square brackets, we typically use to indicate the concentration of that particular compound. This is my equation, if I integrate it, I can then understand, let me integrate it, concentration of A at any particular time t is equal, is going to be equal to A 0 initial concentration k dash t. I want to know when this particular concentration of A at time t is going to be below a particular value.

If I know the initial concentration, then I can get the time because the rate constant, as I mentioned, is constant., that is one way to go about it, not one way, we applied the particular mass balance to our particular system of interest and calculated the variable that we needed, which was time in this case and this kind of closer system, which I just described as a no mass coming in, no moss going out, but which is continuously stirred is called a batch reactor .

Why do I mention this? Because, you do not have the time to, go through such steps, you can look at a particular reactor or a control volume out there in the field and more or less try to classify it as 1 of 3 ideal reactors. The first one, we just discussed batch reactor, the second one will be plug flow or continuously stirred tank reactor and then the plug flow reactor.

Then you will be able to quickly understand how the system is going to behave., the first ideal case reactor we looked at was or is batch reactor. Let us move on and see what else I have out here.

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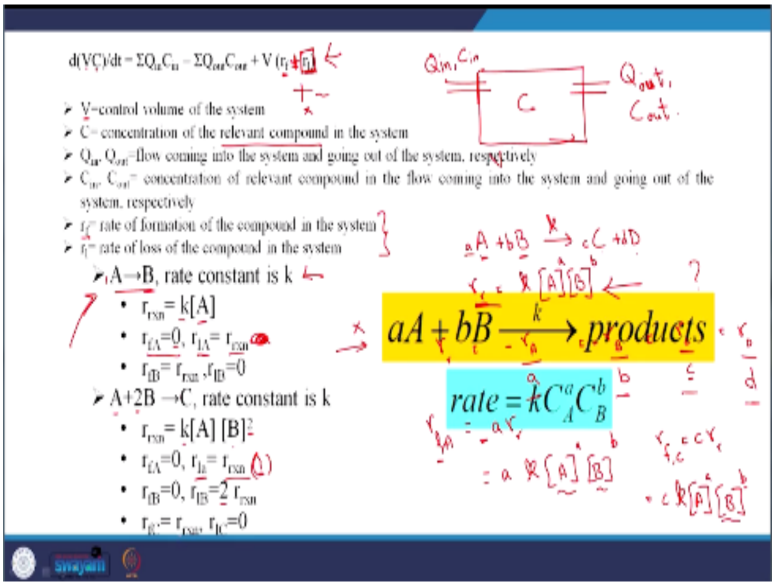

$d(VC)/dt = \Sigma Q_{in}C_{in} - \Sigma Q_{out}C_{out} + V(r_f - r_l)$

- V=control volume of the system
- C=concentration of the relevant compound in the system
- Q_{in}, Q_{out}=flow coming into the system and going out of the system, respectively
- C_{in}, C_{out}= concentration of relevant compound in the flow coming into the system and going out of the system, respectively
- r_f= rate of formation of the compound in the system
- r_l= rate of loss of the compound in the system
  - A→B, rate constant is k
    - $r_{rxn} = k[A]$
    - $r_{fA}=0$, $r_{lA}=r_{rxn}$
    - $r_{fB}=r_{rxn}$, $r_{lB}=0$
  - A+2B →C, rate constant is k
    - $r_{rxn} = k[A][B]^2$
    - $r_{fA}=0$, $r_{lA}=r_{rxn}$
    - $r_{fB}=0$, $r_{lB}=2r_{rxn}$
    - $r_{fC}=r_{rxn}$, $r_{lC}=0$

$aA + bB \xrightarrow{k} products$

$rate = kC_A^aC_B^b$

$$d(VC)/_{dt} = \sum Q_{in}C_{in} - \sum Q_{out}C_{out} + V(r_f - r_l)$$

This is the mass balance equation that you will be using throughout your particular class. Please note that this is nothing but a variation of the fundamental mass balance equation that we already discussed in the previous session., what are the different variables out here just to be sure, we are going to discuss them. V is the control volume of the system.

For example, if this is my reactor in the wastewater treatment plant and flow is coming in and flow is going out and this is the volume of the reactor of interest, and what next? C is the concentration of the compound in the system that I am concerned about. That C is inside the reactor and talking about the concentration of the compound inside the reactor, this C and Q in and Q out, flow rate of the fluid coming in. Flow rate of the fluid going out of the system.

C_{in} and C_{out}, concentration of the compound in the flow coming into the system so, concentration of the compound in the flow coming into the system, C_{in}, inlet C. This should have been out or U_t and then C_{out} is the concentration of the compound in the flow going out of the system C, outlet C. What else do we have? Rate, r_f rate of formation of the compound in the system and rate of loss of component in the system.

Just to refresh your memories with respect to the, what is it now, chemistry here., I have A plus B goes to C plus D, the rate of the reaction is equal to the rate constant rate constant, which is dependent upon temperature and pressure. But typically, temperature, is what we are concerned about assuming the pressure is relatively constant into the product of the concentrations of the reactants.

It depends only on the reactants. Keep that in mind rise to their stoichiometric coefficients. Here, there are no stoichiometric coefficients that is something to keep in mind. But if I transform it such that I have, these are the stoichiometric coefficients. Then what is this rate equation going to be like, k times A rise to its stoichiometric coefficient and concentration of B rise to its stoichiometric coefficient.

As I mentioned, this is the rate of the reaction. But what, how do we relate rate of the reaction to the individual rates of the formation or loss of the compounds here? For example, rate of reaction is what I have. I want to be able to relate that to rate of A, rate of loss or increase or formation of B or C or D. How do I do that? that is by using the stoichiometric coefficients.

That is going to be equal to, by A negative because A is being lost by B negative, and C and D. For example, the rate of loss of A because I am specifying it as loss, I can remove the minus term here, is going to be equal to A into rate of the reaction., that is equal to A into what is the rate of reaction, we have that out here, k times concentration of 8 raised to its stoichiometric coefficient, concentration of B raised to its stoichiometric coercion.

Why A and B? because the rate of the reaction only depends upon the reactants and not that of the products. For example, r c rate of formation of C is equal to C, the stoichiometric coefficient of C times the rate of the reaction., that is equal to C times k into concentration of A raise to stoichiometric coefficient of A, B raised to the concentration, I mean concentration of B raised to the stoichiometric coefficient of B.

You have to be careful about this negative term. For example, when I wrote in the mass balance equation term, here rate of formation minus rate of loss, you should not see to it that you write rate of loss as minus of, some particular equation and you have 2 minuses out here and they cancel out and become a plus that is not what you have. Here, we are writing minus assuming that not assuming because it is rate of loss.

You should not have another negative symbol for the rate of loss and end up having a plus out here. That is something that you have to keep in mind out here. That is why here I did not write rate of loss or such that is why I wrote the negative term here as in, A is being lost, A and B are being lost out here. While C and D are being formed that is why positive out here and negative here.

But because I wrote rate of loss here, I did not use any particular symbol out here that is something to keep in mind., what do we have? We have more or less a review of what we just discussed. A goes to B, rate constant is k, rate of reaction is k times, rate constant k times the concentration of the reactants, which is A. If it is this particular relationship out here, we are going to have rate of formation of A is 0.

Rate of loss of A is equal to rate of reaction times the stoichiometric coefficient that is something that was missing. Rate of formation of B is, rate of formation of B, while, this is not the equation for this particular term. I understand what I was trying to do. This set of information is for this reaction out here and not for this one. Rate of the reaction, this reaction is k times concentration of A.

As we see, rate of formation of A, A is not being formed that is why it is 0. Rate of loss of A is equal to the rate of reaction of A times stoichiometric coefficient of A, which is 1. Rate of formation of B as you see, is going to be equal to 1 times the rate of the reaction. Rate of loss of B is equal to 0 out here. But if it is A plus 2 B goes to C and rate constant is k, what do we have?

Rate of the reaction is k rate constant times concentration of A into B to the power of stoichiometric coefficient, which is 2 out here. Rate of formation of A is 0 because A is only being lost and rate of loss of A is equal to 1 times the rate of the reaction. Why one? Because this stoichiometric coefficient of VA here is 1. That is something to keep in mind. Similarly, rate of formation of B is 0.

Rate of loss of B is the stoichiometric coefficient of B, which is 2 times rate of the reaction. Then rate of formation of C is equal to the stoichiometric coefficient of C, which is 1 times rate of reaction and rate of loss of C is equal to 0 because as you see C is only being formed, it is not being lost. That is something that we have out here.

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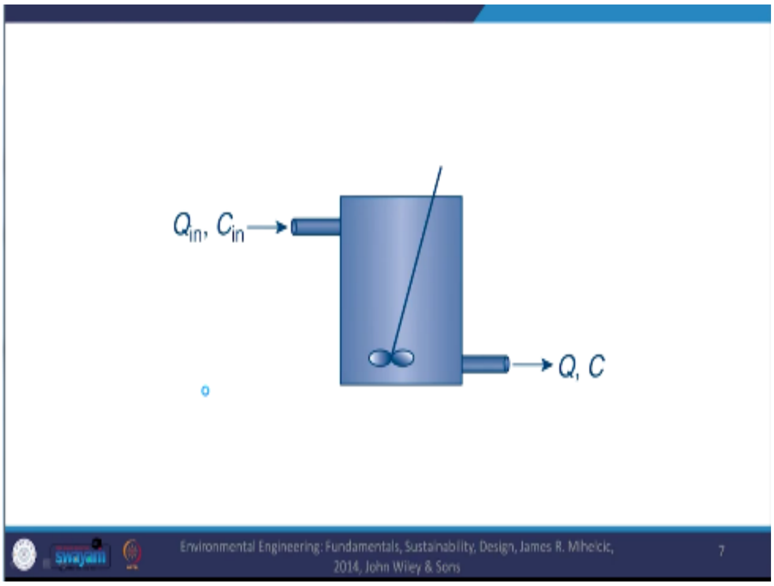

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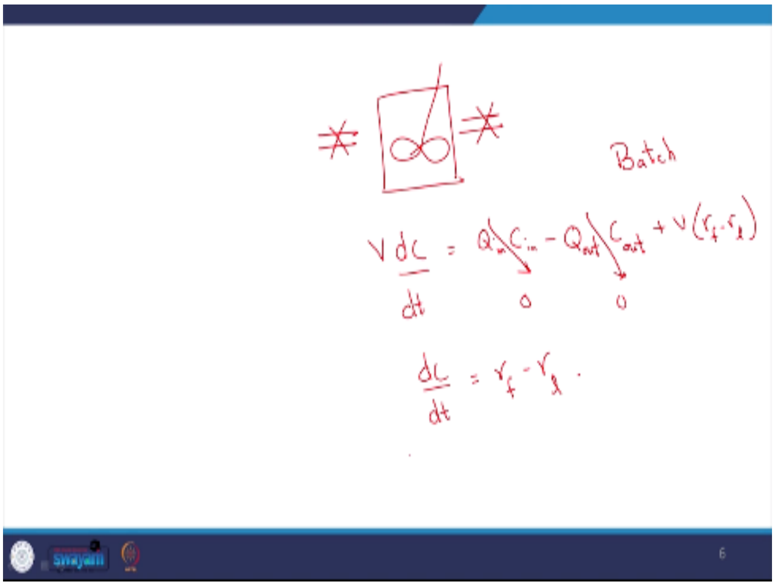

$$V\frac{dC}{dt} = \underbrace{Q_{in}C_{in}}_{0} - \underbrace{Q_{out}C_{out}}_{0} + V(r_f - r_l)$$

$$\frac{dC}{dt} = r_f - r_l .$$

$$\frac{dC}{dt} = r_f - r_l$$

We looked at the case of batch reactor earlier as in, this is my reactor and no flow is coming in and no flow is going out while assuming that it is completely mixed, meaning the concentration of the compound within this particular reactor is the same. For that V dc by dt is equal to mass coming in Q in C in minus Q out C out plus volume into rate of formation minus rate of loss. This is the mass balance equation that we are going to use throughout.

Summation term here, but assuming that there is only one flow, so, these terms turned out to be 0 for the batch reactor. Batch, batch reactor and it just ends up being dc by dt is equal to rate of formation of the compound minus rate of loss of the component. If you have that information, you can solve that.

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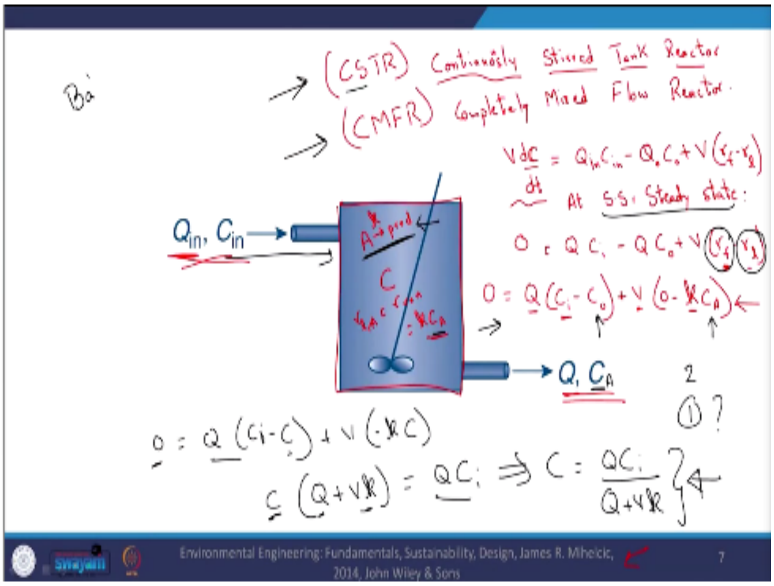

$V\frac{dC}{dt} = Q_{in}C_{in} - Q_oC_o + V(r_f - r_d)$

At S.S. Steady state:

$0 = QC_i - QC_o + V(r_f)(r_d)$

$0 = Q(C_i - C_o) + V(0 - kC_A)$

$0 = Q(C_i - C) + V(-kC)$

$C(Q + Vk) = QC_i \Rightarrow C = \frac{QC_i}{Q + Vk}$

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$$C = \frac{QC_i}{Q + Vk}$$

The next kind of system is modification of the batch reactor as in, we still have continuous mixing, so, the concentration of the compound inside the reactor is the same throughout the system. But unlike the earlier case, we are going to have mass coming in and mass going out. This is from this reference particular book out here, environmental engineering fundamentals sustainability design and design note that, this is a generic figure and can be taken from anywhere or we can draw that too.

But I wanted to mention that reference because that is one of the other, supplementary references you can always look at. We have this particular information. Let us try to apply the mass balance equation to this. When I say this, how do I describe this kind of a system? It is either call continuously stirred tank reactor continuously stirred, it is always stirred tank reactor. It is call CSTR or another name is CMFR as in completely mixed flow reactor.

Both these terms are used to describe this system., the system is that we have mass coming in and mass going out or flow coming in and flow going out and the compound does flow into the system and going out of the system. What is my system? This is the control volume and it is continuously strived or completely mixed always.

Now, let us try to apply the mass balance equation to this particular system out here. We have V dc by dt is equal to Q in C in minus Q out C out plus volume into rate of formation minus rate of loss. We are assuming steady state for the sake of simplicity, but we can always, if the system is not at steady state then this term will not be 0.

What do I understand when I say that system is steady state, it means that if the system is at steady state, all the variables, please note that it is every variable, not just concentration or such, all the variables are constant with time. There is no change any variable in that system with time. If the system is at steady state, that means concentration too does not change with time. dc by dt is going to be 0, assuming that it is at steady state.

At steady state, let me write it down for the first time. Steady, it is steady state is equal to Q in C in minus and one aspect to note is, if the concentration of this particular not concentration, volume of this particular reactor is the same. The fluid volume too does not change with time, then that has to be the case or that will be the case only when Q in and Q out are the same.

Rather than writing Q in, from now, I will just use the term Q . The flow coming in will be equal to the flow going out. Concentration coming in minus Q into concentration going out plus volume into rate of formation minus rate of loss. Let us just try to simplify this a bit more or further. But to simplify this further, if I have no formation but loss.

For example, assume that the compound of interest is being loss by a first order reaction, A is my compound of interest and it is going to products. The rate constant is k. It is not being formed. That is the reaction of concern here., what is it going to be? U is equal to Q times C coming in minus C going out plus volume into, there is no formation of the compound as we just saw 0 minus, how is the compound being loss by this reaction?

What is the rate of loss of this particular compound A? That rate of loss of A is equal to the stoichiometric coefficient 1 times rate of the reaction. What is the rate of reaction? It is nothing but k times the concentration of A within the reactor. That is what I have and that is what I am going to plug in here, is equal to minus the concentration of A within the reactor when I say A concentration of A reactor.

But here, I know the input. I know the flow volume of the system, I will know because the rate constant, I will can get the rate constant. But the issue here is I have only one equation. But I have 2 unknowns as in concentration going out of the system and also concentration of the compound within the system. I have 2 unknowns, but only one equation. How do I solve this?

The issue here is that if you observe the system or if you understand the system, it is continuously shared or completely mixed. The concentration of the compound here within the system is always the same at all locations. What does that mean? The constant once the compound comes in, it is immediately diluted to particular concentration C a.

If the concentration is the same throughout the reactor, what does that mean? That means that the concentration of the compound going out of the reactor is also going to be equal to the concentration of the compound inside the reactor. Why is that? Because if it is completely mixed and the flow is going from the reactor outside to outside the reactor, so, the concentration of the compound leaving the reactor will be the same as the concentration of the compound within the reactor.

With that information, what can I do? 0 is equal to Q into C n minus C out, I will just say C, plus volume into minus k, concentration of compound inside the reactor, I will just say or refer to it as. Now, if I play around with these variables to be able to try to solve for C, let us see, what I will have. I will try to take this term, this term and this term to the left hand side. What will I have out here?

I will have, I will take C as a common term out here. I will have Q plus volume into k is equal to Q into C_i. Hopefully, I did not commit any silly errors. Concentration of the compound leaving the system is equal to Q into C_i by Q plus volume into the rate constant. This is one, we have a first order loss. This is not the case, it is going to be different.

Keep in mind that, how did we end up at this, equation we assumed that first that the system is at steady state, we assume that the compound is not being formed. We assumed that the compound is being lost via first order loss. With that, we ended up with this particular equation. Continuously stirred tank reactor and this is something that we are going to use throughout the class that is for you to keep in mind.

Why is that? If you look at general wastewater treatment plants, which I am going to call by activated sludge process for now, we will understand what it is later. You are going to have our wastewater flowing in to this particular activated sludge tank and wastewater always flowing out and we are going to provide A for the oxygen for the microbes. You are always also going to provide oxygen, which will lead to mixing and more or less same concentration throughout the reactor.

More or less that continuously stirred tank reactor or complete to mix the flow reactor. Please note that it will not always be an ideal reactor but we will discuss this in the next session. Let me just wrap it up., what do we have? We have steady state out here, mass coming in, mass going out and the reaction or the mass being lost by the particular reaction out here.

Taking this terms out to the left hand side and taking C out as the common term. Q minus C comes out here plus, so, I take C, it is Q and V k is equal to Q into C n and end up with this particular system, typically, mugging it up is not a good idea. This class at least whenever I am going to do the, whenever you are going to take the exam, most of the formulae are going to be given.

But if it is simple mass balance equations, I will leave it up to you to be able to solve it. That is something to keep in mind out here. Until now, we looked at the batch reactor and then we moved on to looking at this continuously stirred tank reactor or completely mixing the flow reactor as in unlike the batch reactor, we have mass coming in and mass going out.

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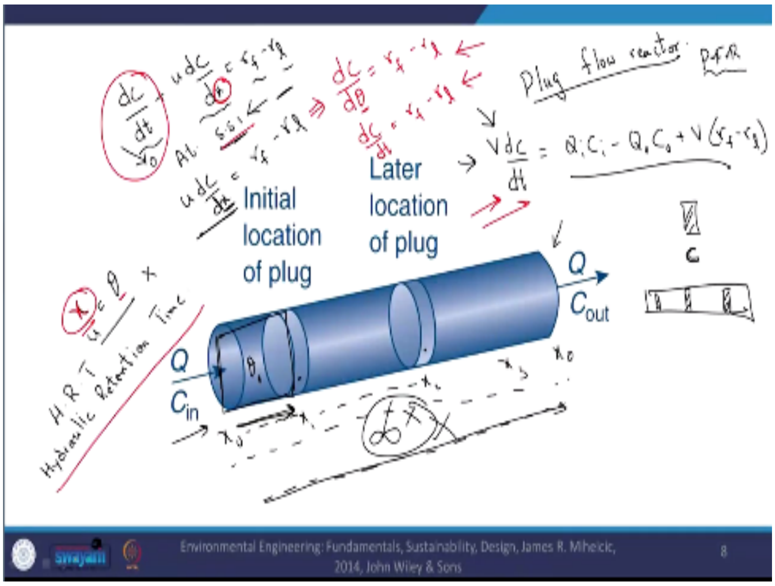

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$$\frac{dC}{d\theta} = r_f - r_l$$

The next one is more or less variation as in we have mass coming in and mass going out. But unlike the continuously stirred tank reactor, there is no mixing inside the reactor. If I, in an ideal case plug flow reactor if I release a tracer here, after particular time and thus distance, I should not say time after particular, after the plug has travelled a certain distance the shape is going to be like this.

Even after x 2 distance after it has travelled x_2, the shape of that plug, original plug will be like this. Why is that? There is no mixing. There is no mixing out here that is why it is called a plug flow reactor. That is something to keep in mind. Within this control volume, so, this particular cylindrical shaped reactor is my control volume. There is no mixing, how does the concentration change?

$$\frac{dC}{dt} = r_f - r_l$$

The concentration changes because as the plug travels along the length of the reactor. It undergoes reaction and it will lead to loss of your particular compound. Let us just try to apply the mass balance equation here and see, what is the issue? Or can I directly apply the mass balance equation V dc by dt is equal to Q_{in} C_{in} minus Q_{out} C_{out} plus volume into rate of formation minus rate of loss.

But, if you look at this equation, here we see that we cannot really apply this equation out here. Why is that? Because, in this system for a first order loss or such, you see that the concentration is changing with distance that say, this is x_0, x_1, x_2 and x_3 and x_{out}. Concentration is changing with distance but in this system, we see that there is no such flexibility.

At least in this equation, the fundamental not fundamental the macroscopic mass balance equation, as we wrote down out here, it is more or less built in for systems within which the concentration of your compound is the same. But here for our plug flow, we see that it is changing out here, it is different out here. The concentration of the compound is changing with distance.

I have to transform this equation, so, that I can apply to my plug flow reactor. We will do that in the next class but as I mentioned, you can always use your fundamental mass balance equation. What was the fundamental mass balance equation, which can be used for every type of reactor with some transformation or the other that is what we have, is equal to rate of formation minus rate of loss.

But here as you see, you have concentration change with time, concentration change with distance and the rates of the different formation and loss reactions. If I want to apply to this reactor or the plug flow reactor PFR, which I call as plug flow reactor, please note that these are all ideal case reactors. What can I do? I can directly apply this particular equation. If it is at steady state, what will it transform into?

This particular term will be 0 and u dc by dx is equal to rate of formation minus rate of loss. But if I look at transforming this further, what is x by u? x is this distance and u is the velocity of flow of this fluid. What will x by u give me an idea about? It will give me an idea about the time, if it is x_1. What does that mean? It spends a time of it, meaning the compound or the fluid spends at time of theta, theta 1 inside that reactor, or it takes a time of theta 1 to travel a distance of x_1.

x by u, I am going to call it as theta or the hydraulic retention time. I will write that out here, hydraulic retention time. It gives me an idea about how much time the particular compound or by conjunction the fluid, how much time the fluid or the compound spends in that reactor x by u. People sometimes think that it is the time that is changing here, it is not.

Keep in mind that the concentration is not changing with time because we already assumed that it is at steady state. The concentration is changing with distance that is what we see out here. That is something to always keep in mind. The concentration at steady state is not changing with time but it is changing with distance. We are only transforming it by writing x, which is a variable and u which is a constant into theta, which is called hydraulic retention times.

What do we get? This rig reaction turns out to be this equation turns out to be dc by d theta is equal to rate of formation minus rate of loss., it is not changing with time. It is changing with distance. Theta is but an approximation of the distance it spends in that travels in that reactor. Theta is hydraulic retention time. Note this similarity with what you had earlier with the batch reactor.

With the batch reactor, what did you have? dc by dt is equal to rate of formation minus rate of loss., you see the similarity hopefully. It is more or less like plug flow reactor is a series of batch reactors, if I may say so. That is it for today, I am almost out of time. In the next session, we will just look at how to transform this macroscopic equation and, applied to this particular plug flow reactor system.

We will more or less end up at this particular point or we will come up with this reaction out here. With that, I will end today’s session. Thanking you for your patience. I will end today’s session.