

Wastewater Treatment and Recycling
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Lecture – 21
Mass Balance: Application in Specific Cases

Hello friends. So, continuing our discussion from the previous lecture when we have started talking about the concept of Mass Balance and how we can use the mass balance within a confined volume which typically is referred as control volume and then analyze the amount of mass which is entering the system, leaving the system or accumulated in the system.

And this class we will see some of the Specific Applications of the Mass Balance in the given different cases how the some basic assumptions or a basic assumptions are considered for applying mass balance to the engineering set ups or engineering systems.

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The slide is titled "Specific Conditions for the Mass Balance" and lists the following conditions:

- **Flow conditions**
 - Batch processes
 - Continuous flow
- **Mixing conditions**
 - Completely mixed systems
 - Plug flow systems
- **Type of contaminant**
 - Conservative
 - Non-conservative
- **Changes with respect to time**
 - Steady State
 - Unsteady State

The diagram shows a 3D white figure standing in the center of a blue, irregularly shaped control volume. Blue arrows indicate mass entering from the left and exiting to the right, with a downward arrow also pointing into the volume from above.

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So, we will be discussing that. To begin with, there are specific conditions in which the mass balance can be applied and at times we need to know these informations ok.

So, what are the flow conditions, whether it is a batch process or continuous flow process; what are the mixing conditions, whether it is a completely mixed system or plug flow system. What are the type of contaminants that conservative or non conservative;

and how it is changing with respect to time, whether it is in a steady state or unsteady state? So, some of these conditions are very important for applying the correct form of the mass balance equation, and how we can simplify the mass balance equation to the given specific cases. So, we will see this one by one.

So, let us see first what all these conditions that we have been talking about implies; we have not discussed some of them earlier.

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Batch Reactors vs Continuous Flow Reactors

- ❖ **In batch reactors**, a batch of reactants are loaded and thereafter allowed to stay till the pre-fixed reaction times. In between, no mass/material is added or withdrawn. Therefore, there is no $m_f(in)$ or $m_f(out)$ in mass balance equation.

$$\frac{dm}{dt} = \underbrace{m_f(in)}_{\text{Zero (0)}} - m_f(out) \pm \frac{dm}{dt}_{\text{reaction}}$$
- ❖ **In continuous flow reactors**, there is a continuous inflow to and outflow from control volume. Therefore, the rate of mass flux in and out has to be considered in mass balance.

$$\frac{dM}{dt} = m_f(in) - m_f(out) \pm \frac{dM}{dt}_{\text{rec}}$$

Image Source: [adapted and modified] <http://cyberfrogdesign.uk/bes/amech/what-is-continuous-process-and-why-is-it-important/>

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So, let us see how this different concept or different conditions that we are we have just been discussing; what they indicate. So, to begin with there are 2 type of reactor, there are batch reactor and there are continuous flow reactors. So, the batch reactor is simply where a batch of reactants are loaded and thereafter allowed to stay till a pre fixed reaction time.

So, you have a tank kind of this you load whatsoever is needed in the system ok; whatsoever reactants needed in the system you load it, you let them let the reaction occur for whatsoever reaction times. So, for say if you want keep it for 2 hours you just keep it for 2 hours there and let the reaction take place. The point here is that in a batch system you have loaded the content in just one single slot; one single batch. And thereafter there is no continuous inflow or outflow from the system.

So, you see there is no like nothing which is bringing in mass, during the reaction is on nothing which is taking the mass out of this system when the reaction is on, so that is what is called batch reactor. So in between no mass or material is added or withdrawn. Therefore, now if you see the classic mass balance equation $\frac{dm}{dt}$ is mass flux in minus mass flux out plus minus change rate of change of mass due to reaction.

So, since there is no inflow there is no out flow. So these terms stands zero and your reaction becomes very simple $\frac{dm}{dt}$ here is equal to whatsoever the rate is changing because of reaction that will only change the content in the reactor, because you do not have any in flow out flow. So, there is no dilution there is no concentration nothing else is happening in the system. So, this is this type of systems are called batch systems or batch reactor. While the continuous flow reactor is when there is a continuous in flow and out flow from the system.

So, in this if this reactor is let us say having in flow which is coming in to the system and continuous outflow which is taking material out of the system. So, then the chemistry or the kind of process that takes place within the reactor changes, there is there is going to be the dilution, there is going to be the other factors coming in. So, rate of mass we can actually estimate the rate of mass flux coming in the system and rate of mass flux going out the system.


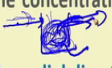
And then these 2 terms are actually exist in our basic equation. So, these do these terms exit and then our classic equation will remain as it is that mass flux in minus mass flux out and plus minus rate of change of mass due to reaction. So, our basic equations here is remains valid whereas, here we will have these 2 terms as 0.




So, these are the batch process or continuous flow process there are something called semi batch process where within the reaction time we can actually keep on adding one parameter or let us say there are 2 reactants needed one we are supplying continuously and one we are putting in back. So, those kind of intermediate process are there which are called semi batch processes those kind of thing. And we can specifically write the mass balance equation depending on which substance which contaminant we are targeting in such systems.

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Completely Mixed vs Plug Flow Systems

- ❖ **In completely mixed reactors**, the content within the control volume remains in completely mixed (homogeneous) state. Such system often needs a stirring device to ensure the mixing in the reactors and are commonly known as **Continuous Stirred Tank Reactor (CSTR)**. CSTRs are simply well-mixed tanks which are used to model well-mixed environmental reservoirs. In CSTRs, the concentration of a substance in outflow remains equal to that in the reactor. 
- ❖ **In plug flow reactors (PFRs)**, the **fluid is mixed in the radial direction, but mixing does not occur in the axial direction**. PFRs are analogous to pipes, typically used to model rivers, canal etc. in which fluid is not mixed in the upstream-downstream direction. In PFRs, each plug of fluid is considered a separate entity, and time passes as the plug flows downstream. Therefore, there is an implicit time dependence even in steady-state PFRs. However, time and downstream distance are interchangeable as usually the velocity of the fluid in the PFR is constant. 

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The next specific case we discussed is completely mixed and plug flow systems. So, what is completely mixed system and what is plug flow system? In completely mixed system as the name itself suggests that the content under the control volume remains in a completely mixed or homogenous state. So, if there is a mixing of the content within the reactor that we call continuously mixed system. So, such system often need a stirring device because how you will mix you have a reactor.

Let us say it could be an; it could be batch processor or continuous flow process. So, you are there is content coming in the system, how you will ensure that the whatsoever is there in the reactor is homogenously mixed? For that you often need a mixing device you need a stirring device. So, that ensures that the content in the reactor is completely mixed.

So, this stirring device is one of the key aspect of a continuously mixed reactor and that is why this reactors are also known as continuously stirred tank reactors. So, the tank where there is a continuous stirring is there. So these are called Continuously Stirred Tank Reactors or commonly pronounced as CSTR. So, this CSTRs are simply well mixed tank there are as we discussed they are mostly they are in the form of tank.

So, they are just well mixed tanks and these are used to model well mixed environmental reservoirs. So, if you are having let us say a lake or those kind of thing where there is a good enough mixing is there, you can use CSTR concept for modeling or in engineering treatment systems; we often design this kind of processes intentionally. So, in CSTR the

concentration of a substance in the outflow remains equal to that in the reactor; so, that is one of the important aspects of this CSTR.

So, what we have is let us say something is coming in from the system and something is leaving the system. So, you may have higher load or this thing coming in the system, but as soon as it enters the system; it gets in to homogeneously mixed and what leaves the system the content that are there in the reactor. So, the water which is leaving the system is actually the water which is inside the reactor and which is homogeneously mixed.

So, when this water is homogeneously mixed and this is the water which is leaving the reactor so; that means, the concentration in the reactor and the concentration in the outlet are going to remain the same ok. So, if a lake is completely mixed and you withdraw some water from the lake or withdraws some water from that through a channel from the lake. So, the water coming in your channel which is originating from the lake will have same qualitative properties as the water within the lake because lake is completely mixed.

So, that is one of the basic assumptions of the CSTR that in the outlet of the CSTR or the amount which is water, which is coming out of the CSTR will have the same pollutant concentrations, same contaminant concentrations as the water in the CSTR. Whereas, the other type of flow reactor is plug flow reactor where fluid is mixed in radial direction only and it does not get mixed in the axial direction.

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Completely Mixed vs Plug Flow Systems

- ❖ In **completely mixed reactors**, the content within the control volume remains in completely mixed (homogeneous) state. Such system often needs a stirring device to ensure the mixing in the reactors and are commonly known as **Continuous Stirred Tank Reactor (CSTR)**. CSTRs are simply well-mixed tanks which are used to model well-mixed environmental reservoirs. In CSTRs, the concentration of a substance in outflow remains equal to that in the reactor.
- ❖ In **plug flow reactors (PFRs)**, the fluid is mixed in the radial direction, but mixing does not occur in the axial direction. PFRs are analogous to pipes, typically used to model rivers, canal etc. in which fluid is not mixed in the upstream-downstream direction. In PFRs, each plug of fluid is considered a separate entity, and time passes as the plug flows downstream. Therefore, there is an implicit time dependence even in steady-state PFRs. However, time and downstream distance are interchangeable as usually the velocity of the fluid in the PFR is constant.

The slide includes two diagrams: one showing a stirred tank reactor (CSTR) with a central stirrer, and another showing a plug flow reactor (PFR) as a pipe with a single fluid plug moving through it.

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So, this PFR or Plug Flow Reactors are analogous to let us say pipe. So, in pipe if you are having a flow ok; so, the water here does not get mixed with the water here ok. Water here will flow and will reach at this place after certain time, but it is not going to mix with this plug or this packet of the water.

So, there is no mixing in the axial direction; mixing can only happen in the radial direction. So, if we are having let us say plug kind of thing this is my plug which is flowing along with the water. So, water within this plug can be completely mixed in a small plug of infinitely small thickness dx . So, if it is a plug of very small thickness dx water in this plug can be in the completely mixed state.

So, because this is basically having a radial mixing, but it cannot get mixed in the axial direction. So, water I mean this plug cannot get mixed in with the water in this plug. So, this is a kind of plug flow system as it happens in the pipes and can be used to model rivers and canals etcetera, rivers we often see that upstream river water and downstream river water will not mix ok.

The water in a upstream of a city and water in a downstream of city where let us say pollutant that being discharged could be drastically different it could be very different. So, in PFR each plug of fluid is considered as a separate entity. So, each plug is a separate entity and as this plug travels within that space the time passes. So, there is an implicit time dependence assumption that it will depend on the time. However, the time

and downstream distance are interchangeable. And generally because in river or even in the particularly in the pipe flow, we consider the velocity more or less constant. So, if velocity is constant we can interchange time and distance ok.

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The slide is titled "Completely Mixed vs Plug Flow Systems". It features two diagrams. The left diagram shows a "Continuous Stirred Tank Reactor (CSTR)" as a rectangular tank with an agitator. It has an inlet on the left labeled $Q(in)$ and $C(in)$, and an outlet on the right labeled Q and C . The right diagram shows a "Plug Flow Reactor (PFR)" as a horizontal cylinder. It has an inlet on the left labeled Q and $C(in)$. A blue arrow indicates the flow direction. Two vertical lines represent the "Initial Location of plug" and "Later Location of plug" at different points along the cylinder. The outlet on the right is labeled Q and $C(out)$. At the bottom of the slide, there is a source URL: <http://www.cee.mtu.edu/~reh/courses/co>. The footer includes the IIT KHARAGPUR logo, NPTEL ONLINE CERTIFICATION COURSES, and the name MANOJ KUMAR, SCHOOL OF WATER, IIT KHARAGPUR, next to a small video inset of a man.

So, that way time dependency can be taken care of. So, if you see in a completely mixed system you will have the sort of stirring device is it is a continuous stirred tank reactor. Whatever is coming in is going out and the concentration here is C ; so concentration in outlet will also remains C , but in a plug flow reactor something is coming on. So, let us say this is the you have one plug here; so this is your initial location at final location this plug will move in the downstream if this is your direction of flow and the concentration here could be different.

So, concentrate the concentration of a contaminant or substance in this time at this plug may be different from this time at this plug and could be different by the time this plug comes out of the reactor. Because it is spending more and more time and the reaction could be taking along with the time progress of the time and that could lead to the decrease in the concentration.

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Conservative vs Non-Conservative Contaminants

- ❖ **Conservative (Non-degradable / Non-reactive) Pollutants**, normally do not transformed to other substances in the receiving water, and tend to be stable and long-lived (persistent). These include, but are not limited to, salts and metals. Since these compounds do not undergo transformation, $(dm/dt)_{\text{reaction}}$ becomes zero.


$$\frac{dm}{dt} = m_f(\text{in}) - m_f(\text{out}) \pm \frac{dm}{dt}_{\text{reaction}}$$

Zero (0)

- ❖ **Non-Conservative (Degradable / Reactive) Pollutants**, are transformed to other substances (generally smaller compounds) through physical, chemical, or biological processes in the receiving water. The rate of transformation depends on the physical, chemical, and biological conditions occurring within the receiving water environment. These primarily include organic matters.




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So, that was plug flow versus continuous flow systems; then we have the type of contaminants which type of contaminants we are dealing with? There are conservative pollutants which are also called non degradable or non reactive pollutants. So, normally these do not transform to other substances in the receiving water because they are conservative, so they conserve their mass; they do not take part in the reaction, they do not get transformed to something else ok.

So, that is what is called conservative pollutant; so these pollutant may include salts and metals which generally do not easily get inverted to other things, they are very persistent in the system. And since these compounds do not undergo any reaction or transformation as the basic idea of conservative or non reactive pollutants are that it will not convert or it will not transform to anything; so, it does not undergo any sort of reaction and its mass rate of change of mass due to reaction is considered as 0.

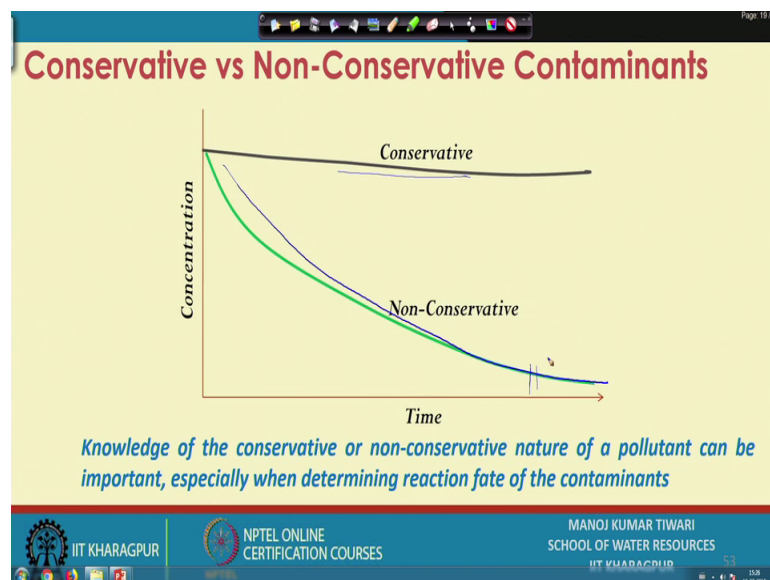
So, in a conservative pollutants we will see that dm by dt due to reaction is 0 and our basic mass balance equation remains this. Rate of change of mass is mass coming in minus mass flowing out ok. So, that is what we lead to the accumulation because there is no reaction nothing is taking place in the system.

It could be non conservative pollutants which are also called degradable or reactive pollutant. The pollutant that can be degraded or the pollutant that is reactive and that reacts undergo a chemical reaction or by a chemical reaction. So, they are generally transform to other substances; normally this smaller substances through various physical

chemical and biological processors ok. And the rate of transformation will depend on the physical, chemical or biological conditions occurring in the receiving water.

So, these are primarily organic matter; organic matters are easily transformable some of the inorganics are also reactive and it take part in the reaction over primarily earning matters are given which are considered as degradable or decomposable stuff. So, for non conservative pollutant your classic mass balance equation is valid, for conservative where this term becomes 0; so, that is what is your conservative and non conservative pollutant.

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Now, if you see; so your conservative is going to retain or conserve its mass while your non conservative with time will lead to decompose and its mass will be reduced.

So, mass reduced means it gets transformed to something else some other form. Now knowledge of whether a substance is conservative or non conservative nature is a very important because as we can set up our reactions or we can set up treatment processes accordingly. So, if you are trying to do a mass balance and you do not know whether the pollutant is conservative or non conservative how you are going to incorporate the reaction term ok.

So, if you want to do mass balance in a better way or in a more efficient economic way; one should know what kind of contaminants one is dealing with.

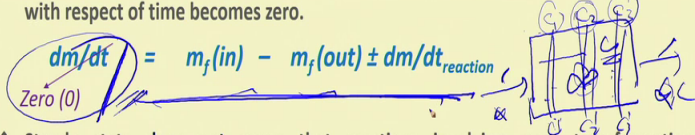
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Steady vs Unsteady State

- ❖ In **steady state**, conditions do not vary with time. Therefore rate of change of mass with respect of time becomes zero.

$\frac{dm}{dt} = m_f(\text{in}) - m_f(\text{out}) \pm \frac{dm}{dt}_{\text{reaction}}$

Zero (0)



- ❖ Steady state **does not** mean that reactions involving mass transformation (degradation) are not occurring, therefore $\frac{dm}{dt}_{\text{reaction}}$ term still remains valid, and contaminant could be degraded with progressing time within the control volume, however, the contaminant concentration (mass) does not change with respect to time in inlet or outlet, or at any given point in control volume.
- ❖ In **unsteady state**, conditions could vary with time at same (fixed) location in the control volume. Therefore, the term $\frac{dm}{dt}$ is not taken as zero.

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Now, another important and specific case is whether the system is in steady state or unsteady state? So, in steady state the conditions do not vary with time; so, rate of change of mass with respect to time becomes 0 rate of accumulation because nothing will accumulate in the system nothing will sort of assimilate within the system.

So, what we have is let us say this is my reactor, this is my control volume. So, we have a inflow coming in, we have a outflow going on. There would be this reaction taking place, but the concentration here or concentration here may remain constant and may not change over the time ok. So, in equation what we get is that rate of change of mass with respect to time becomes 0; when it is in a steady state. There will be inflow there will be outflow, there could be reaction also; so, rate of change of mass due to reaction is not 0; reaction is taking place in the reactor reaction is taking place in the system. But this particularly the rate of change of the mass over the control volume, over the entire control volume is not there ok.

So, that is practically possible; so, this steady state does not mean that reaction is not taking place reaction is there and the mass transformation or degradation is also occurring. So, $\frac{dm}{dt}$ due to reaction is stiller valid term is still taken in the account only thing is that this term is considered as 0. So, the contaminant concentration or the mass does not change with respect to time the inlet or outlet or any given point in the control volume ok.

It can here; obviously, the concentration will be different, here concentration will be different within the control volume depending on whether it is the plug flow system or CSTR. If it is a CSTR, so concentration control volume also remains the same; does not changes. If it is a plug flow system; so, concentration here would different, here would be different, here would be different, but these different concentrations does not change with respect to time.

So, if concentration here is c_1 , here is c_2 here is c_3 ; so, whether we are talking whether we are considering it this hour or may be couple of hours later; the concentration and these locations will still remain the same in a steady state system. Whereas, in a unsteady state system conditions could vary with respect to time and even at the same fixed locations. So, if it is a unsteady state system the concentration here is c_1 , c_2 , c_3 after let us say couple of hours you will see the concentration becomes c_1 prime, c_2 prime, c_3 prime.

Now, these could be a different numbers say in a unsteady system. So, therefore here because the things are changing with respect to times; so, there is a possibility of a accumulation possibility of change of the concentration within the system. So, this term is also not 0; this entire classic mass balance equation remains valid in such cases.

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Reaction Kinetics in Steady/Unsteady State

- ❖ Irrespective of whether the system is in unsteady (transient) or steady state, the transformation reactions occur for degradable (reactive) compounds and their mass is reduced with the progressing times. The rate at which reaction occurs (dc/dt) depend on the reaction kinetics.
- ❖ When this net rate of contaminant mass reduction becomes equal to the contaminant mass inflow, the net mass of the contaminant becomes stable (constant), and the reactor is said to have achieved **Steady state**.
- ❖ The rate of reaction for n^{th} order of reaction kinetics is expressed as $dc/dt = k.C^n$, where C is the concentration of contaminant and k is the rate constant.
- ❖ The first order kinetics ($dc/dt = k.C$) is one of the most popular model for rate estimation in environmental chemistry.
- ❖ A few other kinetic models (e.g. Monod kinetics) are also used depending on the type of reaction and nature of the contaminants.

The slide includes a diagram of a reactor with inflow and outflow arrows, and a handwritten note 'Q.S.' next to it. The footer contains the IIT Kharagpur logo, NPTEL ONLINE CERTIFICATION COURSES, and the name of the presenter, MANOJ KUMAR TIWARI, SCHOOL OF WATER RESOURCES, IIT KHARAGPUR.

Now, if you see the reaction kinetics particularly in a steady or unsteady both the cases; so, irrespective of here system is in steady state or unsteady state ok, the transformation

reactions occurs for degradable or reactive compounds. If it is a non conservative; if it is a conservative compound that term dC by dt due to reaction is anyway getting 0, but if it is a reactive compound.

So, this dC by dC by dt due to reactant will be always be valid or the rate of change of mass dm by dt due to reaction will always be valid. So, this is in particularly in the reaction kinetics if we see the rate at which reaction occur. So, dC by dt is let us say the rate at which the reaction is taking place. So, this rate depends on the reaction kinetics what kind of reaction is there; what is the kinetics of the reaction, it will depend on that ok. So, when this net rate of the contaminant mass reduction becomes equal to the contaminant mass inflow; the net mass of the contaminant becomes stable and we and we say that our system has achieved steady state that is why we do not take that term as 0.

So, let us say due to mass flux in some amount of contaminant is entering in the system ok. So, rate of change of mass here or rate of let us say mass entering in the system here is say any say there is x per unit time ok. And the in the system there is a reaction taking place which is destroying the contaminant which is degrading or decomposing the contaminant. So, let us say in overall control volume if the x amount of the contaminant is getting destroyed in a unit time.

So, what is happening; x amount is entering and x amount is getting destroyed over here right. So, when rate these 2 rates becomes same; the amount which is entering in the system and amount which is destroying from the system becomes same. So, your outlet concentration will also become same; whatsoever outlet concentration unit could be different is, but eventually your outlet concentration will become same means will become stable will not change with respect to time.

Because in unit time whatsoever extra pollutant amount is coming in the system, the same amount is getting destroyed also. So, reaction is taking place in flow is there outflow is also there, but nothing is changing with respect to time. Because in unit time whatsoever amount is coming in that much amount is getting destroyed. So, the concentration have become stable and this is what we call that our system has achieved steady state ok. So, there is reaction taking place, but our system has attained a steady state and this terms becomes constant in that way.

Now, the most like common reaction kinetics which is usually considered is depending on the number of reaction.

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Reaction Kinetics in Steady/Unsteady State

- ❖ Irrespective of whether the system is in unsteady (transient) or steady state, the transformation reactions occur for degradable (reactive) compounds and their mass is reduced with the progressing times. The rate at which reaction occurs (dC/dt) depend on the reaction kinetics.
- ❖ When this net rate of contaminant mass reduction becomes equal to the contaminant mass inflow, the net mass of the contaminant becomes stable (constant), and the reactor is said to have achieved Steady state. $\frac{dC}{dt} = kC$
- ❖ The rate of reaction for n^{th} order of reaction kinetics is expressed as $dC/dt = kC^n$, where C is the concentration of contaminant and k is the rate constant.
- ❖ The first order kinetics ($dC/dt = k.C$) is one of the most popular model for rate estimation in environmental chemistry.
- ❖ A few other kinetic models (e.g. Monod kinetics) are also used depending on the type of reaction and nature of the contaminants.

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So, if it is a n^{th} order of reaction then the rate of change of mass or rate of change of concentration due to reaction dC by dt is taken as $k C$ to the power n , where C is the concentration and k is the rate constant. So, if n^{th} order of reaction with the rate constant of k will have a dC by dt due to reaction as $k C$ to the power n ; the most common is first order which is most adopted in the literature.

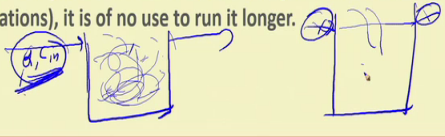
So, for first order n becomes 1 because we are talking about n^{th} order when n is equal to 1. So, we get dC by dt is equal to k to the power k into C and this is one of the most popular model for rate estimation in the environmental chemistry. There are few other kinetic models including like mono kinetics ok, they are also used depending on the type of reaction in nature of the contaminants ok. What kind of reaction we are looking at and what kind of contaminants are there in the system.



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Steady vs Unsteady State

- ❖ Continuous flow reactors usually operate under steady stated conditions, except during start-up when the parameters changes with time (transient state) and tries to attain equilibrium. If flow and inflow contaminant concentration do not change much over the time, the continuous flow reactors will eventually attain steady state and could be operated in the steady state for long.
- ❖ On the other hand, batch reactors are intended to operate under kinetic conditions, and are stopped as soon as equilibrium is achieved. As there won't be any further mass transfer or decay post equilibrium in a batch reactor (due to lack of reactants or physicochemical limitations), it is of no use to run it longer.





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So, formally the continuous flow reactors usually operate under a steady state conditions. Because once you start reactor continuous flow reactor; so you are particularly if there is a let us say discharge or in flow concentration are more or less same. If they do not change with respect to time; so, you are you have started entering putting in this in the system. So, during the starter process when you began the reactor there might be some fresh water or something or the how they degradation or decomposition takes place there might be the bacteria.

So, during the start up the parameters will; obviously, change with respect to time. So, during the startup it will be in the transient state ok, but eventually over the period of time it will attain equilibrium. So, if flow and in flow if like the discharge and in flow have a contaminant concentrations do not change with respect to time; the continuous flow reactors will eventually attain steady state and then they will operate in a steady state ok.

Because with this fixed inflow at fixed rate; you cannot have always changing conditions over here at some point of time this reactor is bound to get in a stable state, in a static state and then we say that it has achieved a time steady state. On the other hand, the batch reactors when we see they are intended to operate under kinetic conditions. Why; because we do not have any inflow or any outflow of the contaminant during the reaction time.

So, all is happening in the reactor is there is a reaction happening and which is changing the level of contaminant with respect to time. So, by the time it changes the level of contaminant with respect to time.

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Steady vs Unsteady State

- ❖ Continuous flow reactors usually operate under steady stated conditions, except during start-up when the parameters changes with time (transient state) and tries to attain equilibrium. If flow and inflow contaminant concentration do not change much over the time, the continuous flow reactors will eventually attain steady state and could be operated in the steady state for long.
- ❖ On the other hand, batch reactors are intended to operate under kinetic conditions, and are stopped as soon as equilibrium is achieved. As there won't be any further mass transfer or decay post equilibrium in a batch reactor (due to lack of reactants or physicochemical limitations), it is of no use to run it longer.

The slide includes two hand-drawn diagrams. The first diagram shows a rectangular tank with a vertical arrow pointing upwards from the bottom, representing a continuous flow reactor. The second diagram shows a rectangular tank with a horizontal arrow pointing to the right from the left side, representing a batch reactor. The slide footer contains the IIT Kharagpur logo, NPTEL ONLINE CERTIFICATION COURSES, and the name MANOJ KUMAR TIWARI, SCHOOL OF WATER RESOURCES, IIT KHARAGPUR.

So, if let us say this is my batch system; then initially my concentration is here and with respect to time it is decreasing. So, I will be interested only to operate this system as long as this concentration is decreasing; let us say beyond this point it has stabilized.

So, this system has attained equilibrium beyond these points; so, no more changes are happening with respect to time. But if I keep my system still on; it is just a waste of time and waste of resources because whatsoever degradation or decomposition has to be there has taken within this much of time. So, we want to run the batch reactors for this much time only because beyond running beyond this point is not of any advantage.

So, since running beyond this point is not of any advantage for a batch system; what we want is batch systems to run till it attains equilibrium; at attains it attains equilibrium and host that we do not want to run the system ok. Till the changes are significant at time even we can basically discard earlier also till the changes are significant. So in order to optimize this due to when; because beyond this point they will not be any further decomposition or decay, because either due to lack of reactants or due to the physical chemical limitations.

So, it is of no use to run this system any longer and we want to run the batch systems within the stipulated time when this change is with respect to time are taking place the kinetics is that way.

(Refer Slide Time: 28:28)

Mass Balance of Contaminates in Reactors

The diagram shows a rectangular reactor box labeled with volume V and concentration C . An input arrow on the left is labeled Q_{in}, C_{in} and an output arrow on the right is labeled Q_{out}, C_{out} . Handwritten notes include $C \cdot m \cdot L \times V \cdot L$ and $= C \cdot V$.

The central mass balance equation is:
$$\frac{dm}{dt} = m_f(in) - m_f(out) \pm \frac{dm}{dt}_{reaction}$$

Measuring total mass is difficult in environmental systems. Working with concentrations (C) is more feasible.

- Rate of change of mass: $\frac{dm}{dt} = d(C \cdot V) / dt = V \cdot dC / dt$ [considering V constant]
- Mass Flux in: $m_f(in) = \sum Q_{in} C_{in} = Q_{in} C_{in}$
- Mass Flux out: $m_f(out) = \sum Q_{out} C_{out} = Q_{out} C_{out}$
- Nate Rate of Reaction: $\frac{dm}{dt}_{reaction} = V \cdot \frac{dC}{dt}_{reaction}$

Substituting above terms in mass balance equation:
$$V \cdot dC / dt = Q_{in} C_{in} - Q_{out} C_{out} \pm V \cdot \frac{dC}{dt}_{reaction}$$

Footer: IIT KHARAGPUR, NPTEL ONLINE CERTIFICATION COURSES, MANOJ KUMAR TIWARI, SCHOOL OF WATER RESOURCES, IIT KHARAGPUR

So, these are the primary specific cases; now if we see the mass balance of a contaminant in reactor. So, let us say this is our reactor a typical reactor where there is some discharge coming in; there is some contaminant concentration in that. Now, so far we had seen this basically mass balance equation, but measuring the total mass in a environmental system or in a reactor at times becomes very difficult.

So, instead what we do; we work with a concentration ok. If you are having a let us say big size lake or big size pond, big size reactor and you try to monitor the total mass and work with a total mass it becomes very difficult. So, the better is that we just worked with a concentration per unit volume of the water; what is the mass of the contaminant present. So, it is more much more convenient particularly in the environmental system.

So, work with a concentration rather than mass it is much more feasible and much more convenient. So, in such a system let us say the concentration going out is C out flow going out is Q out the volume is V and the concentration within the reactor is for say C . So, if we try to see the rate of change of mass the different terms over here, the first term dm by dt let us say. So, this is what is the total mass in the reactor if my average

concentration is C ? So, C is the concentration means C let us say milligram per liter and V is my total volume.

So, let us say V is the total volume in liter; so, we get total mass C into V into milli gram or gram right. So, C into V becomes total mass; so dm by dt is equal to $d(CV)$ by dt . Now if we assume that the volume is constrained volume of the reactor or volume of the system is constant in natural systems also we can because if we have confined controlled volume. So, we can consider that volume has a constant, you can have a lake or something and we can have approximate that that let us consider the volume is constant. And particularly within engineering reactors or in engineering systems; it is always constant in anyway.

. So, if we consider that volume is constant and then what we get is we can take V out and we get V into dC by dt . So, our dm by dt has converted to V into dC by dt ; the mass flux in the system the mass which is coming in the system now you see. So if there are if this is my system and let us say there are 2 inflows or 3 inflow, here rate is Q_1 , here discharge is Q_2 concentration is C_1 , concentration is C_2 so that way.

So, what will happen that from this particular stream; how much mass is entering in the system? If what is Q ? Q is the discharge, discharge means amount of water entering for unit time. So, in a given time how much water is entering in the system right that is what is the Q and in the water which is entering what is the level of contaminant in that? So, it is basically let us say meter cube of per second is our discharge meter cube per hour.

So, in 1 unit time, in 1 second how many meter cubes of water has entered in the system and what is the concentration of the contaminant in that water. So, consider contaminant concentration will be milligram per liter ok, you can convert this meter cube to liter also; so liter per second into milli gram per liter. So, we will get cancelled and what we get is milligram per second. So, rate of milligram per second of milligram per second or milligram per means mass per unit time.

So, rate of change of mass ok; so this is mass flux in right; so units also has to be seen here. So, like here V is in a meter cube this is a constant volume and dC by dt is milligram per liter that way. So, similarly the total mass entering here will be Q in into C in the rate of mass flux in and if there are more than one; so we will have a summation of that ok; sum of all these streams Q in Q_1 into C_1 plus Q_2 into C_2 plus Q_3 into C_3 .

If there is just only one; so, Q in into C in; so this becomes mass flux in and similarly we get mass flux out as Q out into C out summation of right. So, that is how we will get the rate of mass entering in the system and rate of mass leaving in the system. Rate of mass accumulation in the system and then the last term dm by dt due to reaction then also we put in the terms of concentration.

So, as we saw that dm by dt is V dC by dt. So, this will also be V dc by dt but rate of change of concentration here is due to reaction; so V dC by dt due to reaction. Now you can check for the dimension all the terms have should have the same dimension. So, dC concentration in milligram per liter let us say; so we have volume in liter into dC by dt; so, milligram per liter divided by time units; so, let us say second sQ liter per second unit and C milligram per liter ok.

Similarly this one and this also has same unit. So, here you see the liter gets cancel and what units we are getting is milligram per second and same way here also milligram per second. So, the point is mass per second time; so all of these terms, all of these terms have a unit of mass per unit time right and that is what we get.

(Refer Slide Time: 25:08)

Mass Balance of Contaminates in Reactors

Diagram: A blue rectangular box labeled 'V, C' has an input arrow on the left labeled 'Q_{in}, C_{in}' and an output arrow on the right labeled 'Q_{out}, C_{out}'.

$$\frac{dm}{dt} = m_f(in) - m_f(out) \pm \frac{dm}{dt}|_{reaction}$$

Measuring total mass is difficult in environmental systems. Working with concentrations (C) is more feasible.

- **Rate of change of mass:** $\frac{dm}{dt} = d(C.V)/dt = V.dC/dt$ [considering V constant]
- **Mass Flux in:** $m_f(in) = \sum Q_{in} C_{in} = Q_{in} C_{in}$
- **Mass Flux out:** $m_f(out) = \sum Q_{out} C_{out} = Q_{out} C_{out}$
- **Rate of Reaction:** $\frac{dm}{dt}|_{reaction} = V.dC/dt|_{reaction}$

Substituting above terms in mass balance equation: $V.dC/dt = Q_{in} C_{in} - Q_{out} C_{out} \pm V.dC/dt|_{reaction}$

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So, by substituting all these terms over here what we get? Our basic equation changes to V dC by dt is equal to Q in minus u C in minus Q out in to C out. So, this is mass flux in, mass flux out and rate of change due to the reaction. So, this classically gives us the mass balance equation in terms of concentration ok. So, this is the classic mass balance

equation; now we can apply the different the specific cases that we saw earlier, that we discussed earlier to this and do the that kind of vector analysis.

So, we will look that in the next class.

Thank you.