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Lecture – 22 Mass Balance in Reactors: Analysis and Practice Problems

Hello friends, in the previous 2 classes we have been discussing about the concept of mass balance and how it can be applied to specific cases, which we discussed in the earlier class. So, in this lecture we will be talk seeing it is application and it is analysis in the reactors and how we will take some of the practice problem also to solve that.

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So, the mass balance in when we talk about in the different reactor. So, let us say in a continuously mixed system which is CSTR. So, how mass balance is applied in a CSTR we have our classic mass balance equation ok. That we know that your V dC by dt is equal to Q in to C in minus Q out in to C out and plus minus P dC by dt due to reaction.

So, in a CSTR when let us say the rate of inflow and outflow is the same. So, your Q in Q out remains the same. So, this remains as Q, if in CSTR we have said that, what so ever is the content in the reactor that is what is going out from the system. So, the concentration coming out from the reactor and concentration in the reactor are going to remain same. So, then your C out is actually equal to the concentration in the reactor which is C ok. Now if we consider it say order of reaction as n and rate constant k. So,

then dC by dt is equal to k C to the power n as we discussed earlier. So, our final mass balance equation reduces to V dC by dt is equal to Q into C in minus Q into C, because C out is actually equal to C and plus minus V in to k C to the power n. Usually this will be minus because if you are talking about decay.

So, usually this is going to be the minus and this becomes our final mass balance equation for a continuously mixed system. Now again depending on the specific and special cases if we are seeing at, let us say steady state and first order decay. So, in a steady state what will happen; this term will turn 0, so this side will become 0. We will have Q into C in minus Q into C, and if it is a first order decay. Decay means minus V into k into C ok. And this equation can be rearranged to this form. So, C becomes C in 1 divided by 1 plus k V to the power Q k V by Q ok.

If it is a unsteady state conservative pollutant initial concentration 0. So, this case we are have we are talking about a unsteady state and a conservative pollutant. So, conservative pollutant means reaction terms becomes 0 and unsteady state means first term will be there. So, we will have V dC by dt is equal to Q into C in minus Q into C because it is a CSTR. So, this is going to remain C or C out are same actually and there is no reaction term. So, that term is 0 ok, if initial concentration is 0, so or the incoming concentration is 0; then we can sort of get a specific case of that.

Unsteady state first order decay rate constant k no inflow concentration. So, if it is a unsteady state, we have V dC by dt. If it is a first order decay, so reaction term is also going to be there no inflow concentration. So, if there is no inflow concentration, so we have seen our Q in actually 0. So, 0 minus Q into C out or C and minus V k in to C with the first order decay. So, this kind of this will lead to this so we can actually based on the specific cases we can derive these a specific cases.

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In a plug flow system ok, the mass balance for a plug flow system will be again we can work it from the basic principle. So, how is plug flow system? Let us say you are having a plug flow reactor like this, where there is a flow coming in. The concentration in flow in the inflow is C in flow leaving out the discharge remains same, but the concentration is C out ok. And remember so the concentration there is no unique concentration here, because concentration in a plug flow system will be different at different places. As the plug progresses the concentration will change concentration is a function of space or function of time ok, it is not the same.

So if we do a mass balance for let us say this plug we have this plug say the thickness of the plug is dx. And the concentration at inflow is x or 1 boundary of plug is x and the concentration at other means the distance at other boundary is x plus dx so, that thickness becomes dx.

So, concentration here is a function of space, so this becomes C x and concentration here becomes C x plus dx right? So, if we try to apply a mass balance for this plug only so what we have? V dC by dt ok, Q into C x; Q is the flow is the same everywhere across this boundaries also the flow remains same Q. So, Q into C x the concentration entering in the plug minus Q into C x plus dx the concentration that is leaving the plug and plus minus V dC by dt due to reaction ok. Now this if this is let us say assume a steady state so this term becomes 0, when we consider this as a steady state and we can take this out.

So, taking both these terms toward the right side we get Q C x plus dx minus Q C x is equal to this is due to reaction.

Now we can take the Q out from here, what we get? C x plus dx minus C x and here we can write volume of this plug what will be the volume of this plug, if the cross sectional area is a and thickness of the plug is dx.

So, V is going to be equal to a into dx right? So, we will write this as a into dx and d C by dt due to reaction. So, we can take the Q this side and dx this side. So, what we get C x plus dx minus cx divided by dx is equal to plus minus a by Q dC by dt due to reaction. And from the classical calculus we know that cx plus dx minus C x by dx is actually dC by dx. So, what we get; the expression is dC by dx is equal to a by Q dC by dt due to reaction and if it is a first order decay. So, this becomes minus a by Q into k C ok. And this equation will eventually turn as C is equal to C in means; we can we can convert this equation to like this. So, dC by dt dC by C is equal to minus k A by Q into d x.

Now if we integrate this, this becomes ln C and here it becomes x. So, minus k A by Q into x ok, we can we can have the integration coefficients also. So, if we integrate this, let us say to the entire length of the reactor if the total length of the reactor is let us say L this plug flow reactor.

So, x varies from 0 to L, if let us say my this is 0 point and this is L point. So, x varies from 0 to L and C varies from C in to C out, concentration here is C in concentration here is C out ok. So, what we get from here; is actually if you see. So, from this what eventually we will get ln C out minus ln C in is equal to minus k A by Q into your x, x has a range from 0 to L. So, this will become L minus 0 ok.

So, this will be minus k A by Q into L, L minus 0 is equal to L and this will be ln C out by C in right? So, what happens here that A into L is the total volume of this reactor. A is a cross sectional area and L is the length. So, A into L is the total volume of the reactor earlier we consider the volume of plug. So, we took a into dx, now we are considering the volume of the total reactor. So, that is going to be A into L, so A into L will become volume so we have k V by Q instead and ln can be taken here as exponential power.

So, what we get C out by C in is equal to exponential of or e to the power minus k A into L becomes V by Q right? Or C is equal to C in exponential of k V to the power Q, and V

by Q is actually the time till what it remains in the reactor. So, we can say that at time t, so it is actually C in e to the power minus k t ok which is a standard typical first order derivative. So, that way we can do it for a plug flow reactor also and then we can do in a sort of batch system also we can apply.

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Mass Balance: In a Batch 5	ystems	
In batch systems, the rate of inflow and out flow is	s zero ($Q_{in}=Q_{in}=0$). Substituting the terms:	
$V.dC/dt = Q_{in}C_{in} - Q$	$pur \mathcal{E}_{out} \pm V.dC/dt _{reaction}$	
The mass balance equation reduces to:	$V.dC/dt = \pm V.dC/dt \mid_{reaction}$	
0 For n th Order decay at rate constant k :	$dC/dx = -kC^n$	
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So, in batch system the rate of inflow outflow is 0. So, we can substitute this in a classical equation and what we get here is these terms turns out to be 0. So, we have V dC by dt is equal to plus minus V dc by dt due to reaction and dC by dt is equal to minus k to the power C n. If it is a first order so it become simple dC by dt is equal to minus k into C and C is equal to C naught e to the power minus k t.

So, that becomes the case for a batch reactor also ok. So, that way we can apply the concept of mass balance to some of these practical, some of these kind of setups, practical setups whether it is a continuous flow system batch flow system or whether it is a completely mixed system or plug flow systems.

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So, let us take a look at what are the different applications for this mass balance in wastewater treatment. So, the wastewater treatment essentially targets the removal of mass of various contaminants present in it that is, what is the basic objective of the wastewater treatment? What it tries to remove the mass of the contaminant so that; water can be clean or purified. So, that the concentrations could be lower to the level of desired limit, that is the major objective. Now it is important to have an understanding of how this contaminant mass is getting removed or getting reduced and where it is going. And this kind of information this kind of information we can only obtain through a detailed mass balance.

So, for what is ever a specific contaminant we are considering in, we must take that contaminant into account and try to observe it is all entry route, exit route and what is ever happening in between to that contaminant. And that way we can through it is proper mass we can assess it is the fate, it is different fate and transport processes in detail. The concept of mass balance is also widely used for the design and optimization of various treatment unit.

So, if you are planning to let us say design a simple reactor system for our treatment biological systems, depending on the reaction rate how much contact time you would like to give. So, how much mass should we bring in to that system, what should be the sizing, so we can do the sizing or design of the reactor based on that, if you are trying to let us say a physical settlement you need.

So, how much time it will take for the mass to settle down and how much mass is actually getting settling down. So, what should be the volume of that zone, what should be the volume of the different zones of a settlement unit all those things. So, the like this design and optimization is largely depends on the concept basic concepts of mass balance, it is also used to predict the degree of treatment or the finally, fluent concentration.

So, like we were just seeing that from a reactor what is the final C? So, if we know that in input C, if we know the reaction rate constant if we know the size of the reactor we can determine or we can model, we can predict what would be the final concentrations. So, that way we can predict the final effluent concentrations or degree of treatment which is basically C by C naught ok. So, to what degree or what efficiency the system or reactor is working that also we can determine based on that. This concepts can also be used for assessing to what extent the pollutant removal is possible. And whether there are intermediates or byproducts going to accumulate in the system or these the chemical or biological transformation that are taking place.

So, how effectively to what extent this can happen whether this is going to go to complete mineralization scale or if there are byproducts are being formed. What are the mass of the byproducts that will be formed, whether they are the; these byproducts we can do a mass balance for these byproducts to know whether there will be accumulating in the system or they are getting decomposed to further daughter products. So, all those kind of analysis is also possible with the mass balance.

So, there are variety of applications and we will from time to time see in the future lectures when we go on to discussion of the different specific units of the wastewater treatment; however, to start with let us see some quick simple practice problems, how this concept of mass balance is applied. Many time we solve problems using concept of mass balance, but we do not realize that what essentially we are doing is mass balance ok.

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So, far say the dilution how much mass is coming in the system how much mass is going out of the system or what is happening after the mixing, that that also is a problem of. In fact, a mass balance only ok. So, those kind of many problems we solve so we will take a look at some of the simple problems quickly. So, the first problem is on the first order rate constant. So, a pollutant is following first order decay in a lake and it is half life is determined to be one 20 days. So, we need to calculate the rate constant and the time required to achieve 10 percent of initial concentrations.

So, it is a lake pollutantees a in a lake, so we can consider that lake to be let us say well mixed system ok, consider that lake to be nicely mixed system and we can consider that as a kind of batch problem, because there is no information given whether there is any inflow or outflow from the lake. So, if this is my lake and there is no other in no other input or output is provided, what all information I have that there is a first order decay of a contaminant is taking place in a lay lake and it is half life is given as 120 days ok.

And we need to determine the time that will require to achieve 10 percent of it is initial concentration right. So, if we apply again let us this is a batch process right, so in the classical mass balance equation dC by dt is equal to Q in into C in minus Q out into C out plus it is a decay problem, so minus V dC by dt due to reaction ok. So, these terms become 0 this terms become 0 ok. And this V gets cancelled that way what we get is dC

by dt is equal to minus dC by dt due to reaction, which is first order reaction ok, because it is a first order decay that is information is provided to us.

So, we have simple equation dC by dt is equal to minus k into C ok. And this equation can eventually be solved as C is equal to C naught e to the power minus kt right, that is fairly simple ok.

So, this is our final governing equation, C is equal to C naught e to the power minus kt for this lake ok. And we know that half-life means the concentration has turned half in the time in which the concentration has termed half. So, at t is equal to 120 days we get C is equal to C naught by 2 or 0.5 C naught. So, we replace that here, so 0.5 C naught is equal to C naught e to the power minus k into 120 days. C naught gets cancelled and if we take log of this. So ln 0.5 is equal to minus k times 120. Or from here we can get k is equal to minus log of 0.5 ln of 0.5 divided by 120.

So, from here we can determine the k and then once we know the k. So, we can again use what has been asked that how much time it will take to achieve 10 percent of it is in itself concentration, means; we need to determine time when C becomes 0.1 times of C naught just 10 percent of C naught. So, we can further substitute this in the same expression and we will get 0.1 C naught is equal to C naught e to the power minus k times t. And this t here is unknown to us, but k we have determined from here ok. So, this C naught gets cancelled it is only unknown is k.

We can take the again ln here, so ln 0.1 is equal to minus k times t or from here we get t is equal to minus ln 0.1 divided by k. So, we can determine k from here we can substitute this k and we can determine the t. So, that gives us the this gives us the rate constant and this gives us the time required to achieve 10 percent of concentration.

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Practice Problem: First Order	Rate Constant
➢ A pollutant is following first order decay in the lake wate	r and its half–life was determined to be 120 days.
Calculate the rate constant and the time required to achi	eve 10% of its initial concentration.
Let's consider the lake as batch system as no inflow ar	nd outflow information is provided.
For first Order decay at rate constant k:	$dC/dx = -kC \rightarrow C = C_0 e^{-kt}$
Half life is 120 days, i.e. <i>C</i> remains <i>C</i> ₀ /2 in <i>t</i> =120 days.	$C_0/2 = C_0 e^{-k(120)}$ $1/2 = e^{-k(120)}$ ln (1/2) = -k (120) $k = - \ln(0.5) / 120 = -(-0.693) / 120 = 0.693 / 120$ Rate constant, $k = 0.00577 d^{-1}$
Time required for achieving 10% of its initial concentration ($C = 0.1C_0$) is say t. $0.1C_0 = C_0 e^{-0.00577(t)}$ $t = -\ln(0.1)/0.00577 = 399 \ days$	
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So, it is a, that is how we can determine this is a solution of the one in the line that we discussed. So, we have eventually k is equal to minus ln 0.5 by 120. So, this is turning out to be 0.00577 per day, that is our rate constant and then once we have 0.1 C naught is equal to C naught e to the power this, so this gives us t is equal to minus ln 0.1 divided by k and this gives us 399 days.

So, in 399 days we are expected to have the 90 percent removal and only 10 percent will remain in the system with the rate constant given to us.

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So, let us take another problem which is decay in a steady state CSTR and PFR. So, how this happens, we have a 400-meter cube CSTR which receives water from a single inlet ok. So, if you see we have a let us say CSTR which receives water from a single inlet, there is a single inlet and there is flow 40-meter cube per hour. And the volume of the CSTR is 400-meter cube ok. And this the inlet flow is considers 20 milligram per liter of TPAH. There is contaminant now we need to determine the steady state TPH concentration in the exit stream. So, if it is in a steady state; obviously, the flow will remain the same.

So, 40-meter cube per second is the per hour is the outflow also and we need to determine what is the concentration here in the single out outlet ok. The k value is given to us further it says that what should be the volume of a corresponding PFR this is a CSTR, and then what should be the volume of corresponding PFR; if the same like with same inflow same kind of reaction rate constant, what comparative volume of PFR we can use to get the same outlet concentration.

So, first step is to determine the concentration in the outlet ok, which is we will be doing by doing a mass balance in the CSTR that is the first step.



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So, if we do a mass balance in the CSTR our generic mass balance equation is this, now this problem says that it is a steady state ok. So, because we need to determine the steady state, so there is a steady state assumption; that means, this term becomes 0 in a steady

state assumptions it is a CSTR, so C out is equal to C, and it is a first order decay so this becomes kC. So, our equation reduces to 0 Q in into C in minus Q into ck. So, from here we can rewrite it as Q plus kV into C is equal to Q by C in. And eventually we get C is equal to C in one divided by 1 plus k V by Q ok. So, this TPH concentration final concentration from that CSTR will be like this. So, our initial C in is 200 milligram per liter into one divided by 1 plus k value 0.27 per hour and V is 400-meter cube and Q is 40-meter cube per hour.

So, this becomes 10, 2.7 plus 1 3.7 so 1 by 3.7; that means, 5.4 milligram per liter is the final concentration that is coming out of the CSTR. Now what happens like if we want this same concentration 5.4 milligram per liter to come out of a PFR.

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What corresponding volume of PFR should be used? So, for plug flow system again this is our generic mass balance equation, so plug flow system is also in a steady state ok. So, in a steady state this terms become 0 and it is a first order decay, so this terms again become your as k into C right. So, this equation reduces to Q into C in minus Q into C out V into k into C, and as we discussed for plug flow in a steady state earlier, so we get final expression as C out is equal to C in e to the power minus k V by Q. Ok or V by Q we can write as t also so that will be C in e to the power minus k into t what is ever form we writing.

So, for same degree of treatment; that means, our C out has to be kept 5.4 milligram what we obtain for CSTR. So, for that we need to see, so since this is our final expression we can put in here, so we can solve that we can take C out by C in and take ln. So, we get minus kV by Q. And from here we can get V is equal to here Q by k into ln C out by C in.

So, our Q is this much k is this much Q by k into ln C out by C in. So, C out we have to keep the same and C in was 20, so this becomes 194-meter cube. So, this what we can see here is that; for the same degree of removal a CSTR required 400-meter cube of volume, how your plug flow can achieve that volume in a much smaller size almost half of that less than little half of that. So, 194-meter cube, so plug flow systems that we are more effective from reaction prospective; however, there are limitations of the mixing and temperature control and other things. So, both CSTR and PFRs are used actually in practice or in the field ok. So, this is how we can study the decay in CSTR and PFR.

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Practice Problem: Unsteady State	
> A 500 m ³ size CSTR pre- filled with clean water started receiving water from a waste stream containing	1
100 mg/l of a conservative pollutant at a flow rate of 50 m³ /day. An outflow channel was also started	
simultaneously to ensure the passage of extra water in the pond. Calculate the pollutant concentration i	1
the outflow as a function of time after start?	
Generic mass balance equation: $V.dC/dt = Q_{inr}C_{in} - Q_{out}C_{out} \pm V.dC/dt _{reaction}$	
For a CSTR ($C_{out} = C$) with conservative pollutant $dC/dt _{reaction} = 0$; $V.dC/dt = QC_{in} - QC$	
$dC/(C_{in}-C) = (Q/V).dt$	
$ln(C-C_{in}) = -(Q/V).t + I$	
Initial condition: at $t=0, C=0; \ln(0-C_{in}) = -(Q/V), 0+1 \rightarrow 1 = \ln(-C_{in})$ $\ln(C-C_{in}) - \ln(-C_{in}) = -(Q/V), 0+1 \rightarrow 1 = \ln(-C_{in})$.t
$\ln(C-C_{in}/-C_{in})=-(Q/V).t$	
$C - C_{in} / - C_{in} = e^{(Q/V).t}$	
$C-C_{in}=-C_{in}e^{(Q/V).t}$	
$C = C_{in}(1 - e^{(Q/V),t}) = 100 (1 - e^{t})$.11)
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We will take just one more problem, in the last problem which is on the start up of a CSTR ok.

So, start up as in when we are talking about this as a start up. So, it is actually becomes unsteady state problem. So, we have a 500-meter cube CSTR pre filled with clean water started receiving water from a waste stream containing 100 milligram per liter of a conservative pollutant. So, we are having a CSTR ok, this is of 500-meter cube size, so volume is given to us. And this is pre filled with the clean water and it is a started receiving a waste which is containing 100 milligram per liter of a conservative pollutant at a flow rate of 50-meter cube per day.

An outflow channel was also started simultaneously, because it is pre filled with the water and so once the water starts coming in the same amount of water we will start leaving in also. So, the flow rate remain same Q out remain same 50-meter cube per day. Calculate the pollutant concentration in the outflow as a function of time after start remember this is a conservative pollutant, so there is no reaction term here.

So, dC by dt due to reaction here is actually 0 being a conservative pollutant. So, in a in your classical mass balance equation again we can apply the basic principle basic concept of the classical mass balance equation. And see how we can simplify that to derive what is ever information we need. So, our generic mass balance equation is this, now for a CSTR we know that C out is actually equal to C and there is no reaction, so this term become 0.

So, and it is a unsteady problem because we need to calculate the pollutant concentration as a function of time after starts just at a startup. So, this is actually a unsteady state problem ok, so what happens that our reaction will be V dC by dt is equal to Q in into C in or Q into C in minus Q into C, which is the out concentration there is no reaction that is happening ok. And initially it is in the unsteady state because by the time it reaches a steady state it is a conservative pollutant.

So, what is ever is the concentration in inflow will be the concentration in outflow and reactor because there is nothing which is taking away that concentration. So, this we can rearrange this equation here we can take Q as common. So this becomes Q C in minus C and we can drink C in minus C here, so dC by C in minus C is equal to Q V. We can take this side V by dt we can integrate that now ok, so if this becomes ln C minus C in of course, minus sign can be taken here. So, minus Q V by minus Q by V into t and integration constant, we can apply the initial concentration initial conditions as given ok. So, since the your it was pre filled with the clean water.

So, at time t is equal to 0 there was no pollutant concentration in the reactor. In the control volume the concentration of the contaminant was 0 at time t is equal to 0 because it was prefilled with the clean water. So, that is the initial condition given to us so we

apply these initial conditions we substitute this here so ln, C minus C in instead of C will write 0 minus C in and at time t is equal to 0 so this terms become 0. So, our I or integration constant become ln minus C in. So, this we can substitute I as ln minus C in and can bring in this side so ln C C minus C in minus ln minus C in is equal to minus Q V into t Q by V into t.

So, this we can rearrange like this ln C by C in by C in and this becomes here we can remove the ln and take exponential of this. So, C minus C in by minus C in is this or C minus C in is equal to minus this ok. So, that way we can actually this has to be minus actually ok. So, this way we can have this number right? And eventually what we get is this, and from here 100 is equal to means C inverse 100 so we can substitute C in and Q by V. So, Q was 50 and V was 500 so 50 by 500 is equal to 0.1 so this becomes 0.1 t and this becomes your sort of outflow as a function of time after it starts.

So, concentration in outflow will be like this which is a function of time, C as a function of time that way we can derive for a unsteady case. So, these are some of the problems which can be sort of solved using the concept of mass balance, there are many more the basic concept remains same ok. We will be happy to discuss few more problems in the forum if any of you are attempting or having any query. So, with this we conclude the discussions for this week, this was a little rather long week. And we will start discussing about the treatment of wastewater is specific treatment and what are the different units for the treatment starting from the next week.

Thank you.