

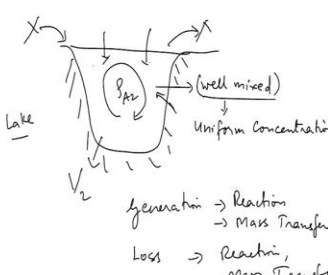
**Environmental Quality:  
Monitoring and Analysis**  
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**Lecture No. 34**  
**Transport of Pollutants - Introduction**

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TRANSPORT OF POLLUTANTS

Objective: Estimate  $S_{A1}, S_{A2}, W_{A3}$  in the environment.



generation  $\rightarrow$  Reaction  
 $\rightarrow$  Mass Transfer

loss  $\rightarrow$  Reaction,  
Mass Transfer


Q: What is  $S_{A2}$  at time  $t'$ ?

Mass Balance of  $A'$

$$\text{Rate of Accumulation} = \text{Rate}_{in} - \text{Rate}_{out}$$

$$= \left( \text{Rate}_{in} \text{ by flow} \right) - \left( \text{Rate}_{out} \text{ by flow} \right)$$

$$+ \text{Rate of generation} - \text{Rate of loss}$$



So, we move on to the next section which is just on transport of pollutants. So, our general idea here transport of pollutants our goal is still the same what we have been discussing right from the beginning the overall scheme of things, is to way are objective is to estimate the concentration rho A1, rho A2, WA3 any of these environment under a wide variety of scenarios. In other words, we are just interested in finding concentration.

As concentration is the main quantity that we are interested in terms of exposure and so, from the chemical moves a pollutant moves from a source to a receptor, what happens to the concentration? It is just such a change, how does it change can we predict it? Can we measure it these kind of things. So, primarily we are looking at modeling of this pollutant transport mainly and then because we have a model we have to we must be able to validate model.

So, we will, use measurement techniques that we learned adapt them to do this in terms of this. So, when we look at transport of pollutants, we look at a very simple scenario at first is the river we will before the rivers a simpler system is a lake. Take a lake, the lake is a fixed volume, there is a fixed volume in the lake and let us say that there is a chemical of concentration fluid to just well mixed.

When we say it is well mixed we are obviously we are assuming that the concentration is uniform. So, if it is well mixed, and let us assume that it is mixing, we will not worry about it how it is mixing, let us assume it mixes it is mixing which means the concentration is always uniform. Now, if I want to predict this is a fixed volume, there is no flow of water there is no flow and no flow of water outside this means that this is fixed volume.

There is a chemical inside here, what is likely to happen to the chemical concentration here so, if we want to question that I will ask is what is  $\rho A_2$  at some time  $t$  in this problem the concentration of  $A$  in this water will only change if it is going away from the system if something is adding or getting lost from the system. So, we invoke our overall mass balance revoke the mass balance of  $A$  in the system.

So, if many of you have done mass balance before the general since the rule the equation for mass balance is rate of accumulation = rate in - rate out this is a general term. Now rate in - rate out can be in different forms. So, here the rating, when we are talking about many general systems we have different possibilities of rate in by flow – rate out by flow – rate in by other processes, rate in rate of this will pretty much cover a lot of processes general processes.

So, in this particular system lakes system there is no rate in by flow, there is no rate out by flow because everything is in the river in the lake normal conditions, the rate of generation or rate of addition into the system by some other form the format some other process so, this rate of generation could be by reaction, which means it is forming by reaction from some other thing or it is coming is transfer is occurring by mass transfer and rate of loss also can be reaction and mass transfer.

Mass transfer means it is going out of the system not with flow by some other means, by evaporation or by accumulating onto the walls of the lakes solid same way this gaining in decision is it is transferring from the sediment to the water or it is coming from air into the water all these are possible. So, the entire mass balance system is written this way.

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General Mass Balance

$$\text{Rate of Accumulation} = \text{Rate in} - \text{Rate out} + \text{Rate of generation} - \text{Rate of loss}$$

↓ Unsteady State  
(Mass of A) / time

$$\left( V_2 \frac{d\rho_{A2}}{dt} \right) = (R_{\text{gen}} - R_{\text{evap}})$$

Evaporation

$-V_2 \frac{d\rho_{A2}}{dt} = R_{\text{evap}}$

$\frac{d\rho_{A2}}{dt} = -v_c$

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Generalized mass balance the general mass balance again. So, the generation and loss there is a sink there is a reservoir and there is a sink this usual terms used for that this is general equation you apply to any system but what we define our system is our main so the rate of accumulation here in the lake for the lake, the rate of accumulation what is the rate of accumulation? The question is this rate of accumulation is if the rate of accumulation exists only when the system is unsteady state.

What we mean by unsteady state, the concentration is changing so, each term in this equation must balance as units of mass of A per time is a unit of rate every term in this unit as rate is a rate term M / A, M / T, MA / T. So, the rate of accumulation unsteady state means it is dA2 / dt multiplied by V2. So, this units are here so, rho A2 is mass by volume V2 is volume and so, this unit is L cube into MA / L cube into time mass by time.

So, for the lake this is 0, and this rate of generation rate of loss could be anything. So if you know what is the rate? At which loss or innovation is occurring that particular process, you have

to put the equation here. So, it could be anything say if it is reaction rate of generation is reaction and this is evaporation, let us say evaporation, I need a term. So now, rate of generation - rate of evaporation so we have we will call it as  $R_{\text{reaction}} - R_{\text{evaporation}}$  which also should have units of mass by time.

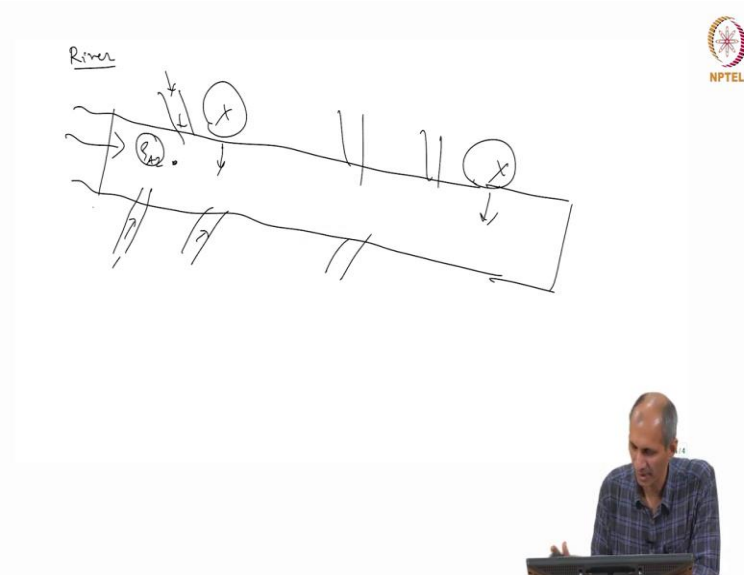
You have look for individual expressions of these 2 terms which comes from other domains of knowledge. So, you know the reaction you know what is the reaction rate system then you the entire thing will come here first order second order equation and so, this the overall signage sign of these things will be there if there is accumulation which means if there is an increase in the concentration of A in the system, this will be positive the left hand side will be positive, it will only be positive if say the rate of generation reaction to formation of A is more than the rate at which it is losing.

So, the sign is important. It could be either way depends this sign of the left hand side depends on what is happening on the right hand side. For example, if we take evaporation only, so the only process occurring is evaporation there is nothing else no reaction. Let us say I have a solution of benzene sitting in a lake. Take a simpler example, if I have a reaction, the benzene sitting in a beaker and I am mixing it, well mixed, the initial concentrations this much from only evaporation is occurring.

This is minus the rate of evaporation the reason I put a minus sign here is that  $d\rho_{A2}/dt$ , if I measuring the concentration, if I measure the concentration of  $\rho_{A2}$  versus time, I am going to start somewhere and because it is evaporating, it is decreasing. So if  $d\rho/dt$  is negative, this is negative rate of evaporation we as we mentioned is positive. Whenever we talk about rate of evaporation, I think this is positive.

So, in order to, make this entire quantity positive, we put a negative sign there. So the general rule of thumb is this if you have loss, there is a decrease in concentration, you put a negative sign to the left of it. To make that quantity positive, the right hand side is always positive, that is a convention we will come to that the exact terms for rate of evaporation, rate of reaction and all that later, but this generally we this is so this is for unsteady state model.

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Now, if you take the case of a river, is long river so you have a big section of river water is flowing and you may have you are interested in getting the quality of water at a given place. Now here you will have different flows coming in from different things. For example, people are releasing waste into water in a river or you are getting sewage into a river, or you may have a tributary that is coming and joining the river, any of these things are possible.

So, the concentration of this depends on what is coming here and what is coming here in each of these channels, and what is evaporating and things like that. So when you write a mass balance, it will be it can be for the entire river. But you also notice that if a material is coming here, and there are 3 sections here, very difficult for me. There is a group of population is lives here and there is a group of population is lives here.

How I model this system for me I need to know what is the concentration at this point? I need to know, what is the concentration at this point? So that I know I need to know, what is the exposure of this set of population whether this set of population? So in order to predict and model, this kind of systems, it is very difficult for me to do this if I have a long system as it is. Here I want to introduce a concept similar to what we did in the earlier system, except that now it is a flowing system.

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Box - Model

Assumptions

1. well mixed (CSTR)
2. steady state

Rate in = Rate out  
 $\rightarrow$  Rate in by flow = Rate out by flow + Rate of reaction

$\rho A_2 \frac{dV}{dt} = \rho A_2 \frac{dV}{dt} + R_{\text{reac}}$

And this this concept is known as a box model. And we will come back to this river system in a minute. We call what is a box model a box model, essentially is it is a box is a 3 dimensional box. It has a certain volume is called it as delta x, delta y and delta z and in this volume, there is a concentration rho A2, rho A1 whatever we call it rho A2 for the time being. The basic assumptions of the box model is that this well mixed the contents are well mixed.

Which means that whatever enters here and something will exit here something can enter something and exit something exit here something enter here, something enter here something exit here all these walls things can enter and exit do whatever they want that is all fixed. But when it says well makes this concentration is uniform throat, there is no gradient or there is no difference in concentration everywhere.

So this would what we call as this when you call it a wellness we use what is called either completely stirred tank reactor or mixed reactor CSTR. This, is the assumption that we make now, if you do this, we also add one more assumption here, because it is a flowing system and this you have a flowing system. You also can make simple superimpose another assumption here which we call it a steady state may not be steady state, but let us have another assumption, relaxing assumption called steady state.

This is very useful in flowing systems because nothing is accumulating everything is moving here so, what can happen here is enter in a river, real river, long river, something enters here, and this concentration may be different from this concentration maybe different from this here for what can be happening is let us say a chemical is entering here. And it can leave it can evaporate. So the concentration is decreasing as it is going if no other addition is happening.

So, how do you predict this concentration here, one way to do it is if I assume that this small section everything is well mixed in here I will I will model what is going out and what is getting out of this system into the next system next box. If I am if I model this as a series of boxes, I make my assumption that this is all uniform inside. So it is easier for me to model if it is uniform in each box. So at one box goes to another box and therefore I can model it very much more easily.

There are other ways to do this. We will get to that in terms of so here if you do a steady state system, there is an accumulation rate in minus rate out. So we add up all these things will say rate in equal's rate out. So we add up all the processes that are contributing rate and so here we will say, rate in by flow equals rate out by flow plus something else you can have rate of evaporation and you can call it as your rate in rate of generation.

So what is happening here is the rate is constant and says this is the same rate that is happening. So what is coming in is going out distributing into 3 difference and let us assume that there is no there is no rate of reaction, let us say only evaporation is occurring. So what is coming in is now going out in as evaporation and I think none of these things are happening. This is being divided into these 2 streams. That is it and the next one goes in there is a different inlet concentration and again, that loss ago.

So, here this is my equation so, if I put this in the form of the sink flow is the rate flow rate of the chemical multiplied by the concentration inlet equals what is going out. Now, the unit of this is this Q is volumetric flow rate, so it is L cubed by T into MA by L cube, this is MA by T this will also be the same. Now, if you notice here, this rho A2 is the concentration that is leaving the

system which is also the  $\rho A_2$  which if since I am assuming it is well mixed, it is the concentration inside this box.

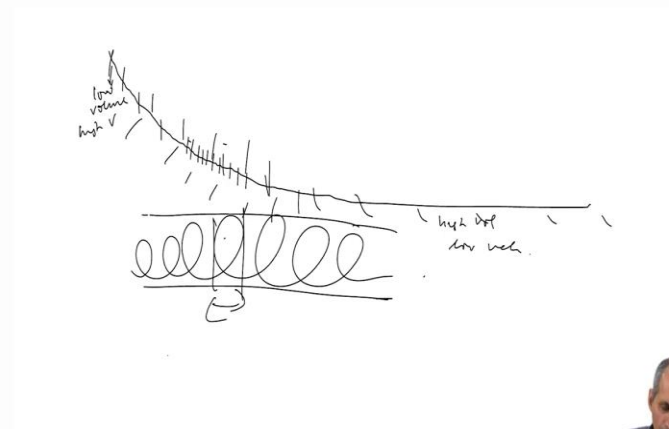
This is a basic assumption of a CSTR. So, well mixed box model. So, into this box model, I can add other terms if I want, I can add other processes that are happening there advantage in the box model if I extend a bunch of box models for put a series of box models there I may have  $\rho A_2$  is 0 that is I have  $\rho A_2$  in there is entering. And here I may have something  $\rho A_2$  is out that is exiting the system.

In between there is a big difference between  $\rho$  in  $A_2$  out in between I am going through a series of individual boxes where something is happening evaporation is happening. They will also possible for me to model this in this as what is called as a plug flow reactor. The same thing I can do as a plug flow reactor I can take small section instead of taking what I am saying is, this is flux flow is going in this direction, this mixing in one zone.

But his progress from one zone to another zone there is a difference because it is losing material reaction is happening on some such thing is happening. So, the reason box model is used in practical systems like the environment is that unlike chemical reaction engineering where blood flow is used for a different remember here it is useful, because the characteristics of each box may be different. For example, if you take the case of a river, if you take the case of river Ganges for example.

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The river Ganges comes from somewhere in the hills, its gradient is like this and then as it comes down to the upper plains and then lower plains it becomes like this. Here the velocity is very high, until it comes here the volume is low here, velocity is high here. Low volume, high velocity here high volume, the lower velocity, the terrain, the nature of the bed of the river is very different in the upper reaches and as we come down into the plains becomes very different.

The cross section of the river is very different, everything is different. So, and there are a lot of tributaries that join and there are a lot of cities that join and all that. So, it is very difficult to predict the quality of water throughout modeling entire, river as one so the segment is divided into a lot of segments. Now, river is flowing very unrealistic to consider river as a well-mixed system because what we consider as well mixed means there is backflow.

I put something here, it goes forward and comes back that may not be happening in a river to a large extent, river. You may have a little bit of back flow because river may flow like this. But this scale of this convection is not very high. But I think a lot of times we do not have a choice otherwise our computation becomes very, very difficult. So, they will generally break it up into this kind of system.

So, the hydrodynamic state of river or water body or the atmosphere becomes very critical to understanding that in order to model these kind of systems. So, if we take the same system, box

model and go to the atmosphere is becomes more the river is very nice. It is a well-defined system. I know the width of river height of the water, I know the volume in each section I know what activity is coming in and all that in the air much more difficult.

You can imagine, if I am looking at air on top of Chennai there is no I do not know what is the dimension of it, I have to assume some dimension. So, this is a much more tricky problem in atmosphere science doing but people have to work on this and we will come to that. So, a box model is use like this. So, what we will do initially now is to in the next few classes, I will look at one box model and the adaptation of box model for water quality, which is a very popular model that is used in for oxygen balance.

And then we will see the adaptation of box models in the atmosphere to look at and then each of these terms that we look at we will look at how it relates to water pollution and air pollution and how it relates to predicting concentrations downstream and all and the assessment and estimation of each of these terms individually in the in the mass balance. The most other systems that we study in the environment are we consider them a steady state except things like lakes.

Where we know that nothing is no fluids coming but lakes also you cannot consider them a steady state in a certain period of time and water is coming in, some chemical and chemical is going out in the form of this thing they have to we have to treat them as separate episodes of this anyway so the idea here behind this thing is you must learn to identify how to take environmental system and put it in the format of a model. So that you can predict or estimate concentrations as a function of time or space, so we will stop here. We will meet on Tuesday.