

**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  $\rho_{A1}$ ,  $\rho_{A2}$ ,  $w_{A3}$  in the environment.

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

Mass Balance of  $\rho_{A2}$

Rate of Accumulation = Rate in - Rate out

$$= \left( \text{Rate in by flow} \right) - \left( \text{Rate out by flow} \right) + \text{Rate of generation} - \text{Rate of loss}$$

Diagram labels: Lake,  $\rho_{A2}$ , (well mixed), Uniform Concentration, generation  $\rightarrow$  Reaction, Mass Transfer, Loss  $\rightarrow$  Reaction, Mass Transfer.

So, we move on to the next section, which is on transport of pollutants. Our goal is still what we have been discussing right from the beginning, our objective is to estimate the concentration  $\rho_{A1}$ ,  $\rho_{A2}$ ,  $w_{A3}$ ; any of these in the 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. As a pollutant moves from a source to a receptor, what happens to the concentration? Is it change, how does it change? Can we predict it? Can we measure it?. So, primarily we are looking at modeling of this pollutant transport mainly and then because we have a model, we must be able to validate that model.

So, we will use measurement techniques that we learnt and adapt them to do this. As we look at the transport of pollutants, we look at a very simple scenario first. Let's take a lake. So, a lake has a fixed volume and let us say that there is a chemical of concentration  $\rho_{A2}$  which is well mixed in it.

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

If there is a chemical inside, what is likely to happen to the chemical concentration here? So, what is  $\rho_{A2}$  at some time 't'? Now in this problem, the concentration of A in this water will only change if it is going away from the system, if something is added or lost from the system. So, we invoke our overall mass balance of A in the system.

Since the equation for mass balance is  $Rate\ of\ Accumulation = Rate_{in} - Rate_{out}$ . Now rate in - rate out can be in different forms. So, when we are talking about many general systems we have different possibilities of


$$Rate\ of\ Accumulation = \left( \begin{matrix} Rate_{in} \\ by\ flow \end{matrix} \right) - \left( \begin{matrix} Rate_{out} \\ by\ flow \end{matrix} \right) + \left( \begin{matrix} Rate\ of \\ generation \end{matrix} \right) - \left( \begin{matrix} Rate\ of \\ losses \end{matrix} \right)$$

this will pretty much cover a lot of general processes.

So, in this particular lake system there is no rate in by flow, there is no rate out by flow, because everything is in the lake at normal conditions, but there is this rate of generation which could be by reaction from some other thing or it is due to mass transfer. Similarly, the rate of loss also can be as a result of reaction or mass transfer.

Mass transfer means it is going out of the system not with the flow but by some other means, for instance evaporation or by accumulating onto the walls of the lakes solid. So, the entire mass balance system is written this way.

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$$V_2 \frac{d\rho_{A2}}{dt} = L^3 \frac{m_A}{L^3 \cdot T}$$

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

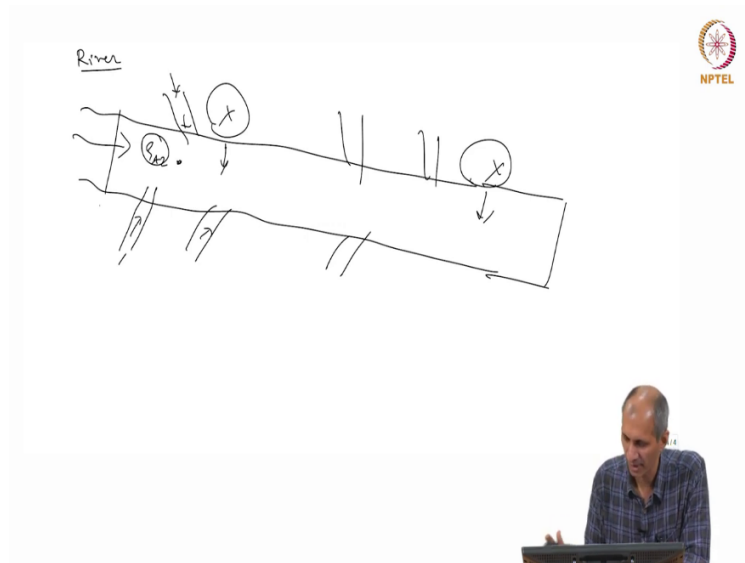
You have look for individual expressions of these 2 terms which comes from other domains of knowledge. So, you know what is the reaction rate, hence the overall sign of the equations formed will be changed. This means if there is accumulation that is, there is an increase in the concentration of A in the system, the left-hand side will be positive, but 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. The sign of the left-hand side depends on what is happening on the right-hand side. For example, if we take evaporation only, the only process occurring is evaporation and there is nothing else (no reaction). Let us say, I have a solution of benzene sitting in a lake. Take a simpler example, in case if I have a reaction, the benzene is sitting inside a beaker and I am well mixing it.

This illustrates a minus sign in the rate of evaporation. The reason I put a minus sign here is that 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 as we mentioned is positive. Whenever we talk about rate of evaporation, 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 and you put a negative sign to the left of it. To make that quantity positive, the right-hand side is always positive, we will come to the exact terms for rate of evaporation, rate of reaction and all that later, but generally we do this for unsteady state model.

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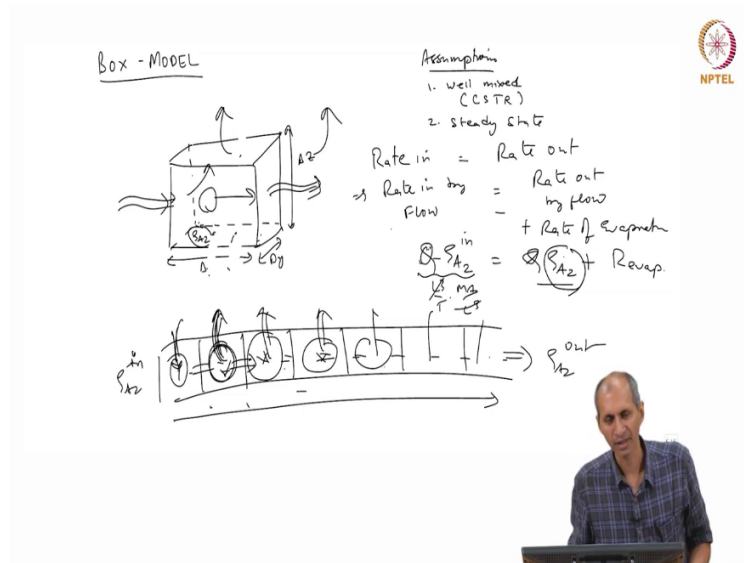


Now, if you take the case of a long river, you have a big section of river water flowing and you are interested in getting the quality of water at a given place. Now here you will have different flows coming in from different things. For example, people are releasing waste into water in a river or you 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 for the entire river. But you also notice that if a material is coming here, and there are 3 sections here, it is very difficult. There is a group of population that lives here and there.

To model this system, I need to know what is the concentration at this point? So, I need to know, what is the exposure of this set of population? So, in order to predict and model, in 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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And this this concept is known as a box model. And we will come back to this river system in a minute. What we call a box model, essentially is a 3-dimensional box. It has a certain volume called as delta x, delta y and delta z and in this volume, there is a concentration rho A2. The basic assumptions of the box model is that the contents are well mixed.

Which means that whenever whatever enters here, something will also exit from here. But when it makes this concentration as uniform throughout, there is no gradient or there is no difference in concentration everywhere.

So, this is what we call as the stirred tank reactor or mixed reactor CSTR. This, is the assumption that we make now. we also add one more assumption here, because it is a flowing system by calling it as a steady state flow.

This is very useful in flowing systems because nothing is accumulating, everything is moving here. So, what can happen here is, something enters here in the river, and this concentration may be different from this concentration which may be different from this. And it can leave or 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 in this small section everything is well mixed, I will model what is getting out of this system into the next

system next box. If I model this as a series of boxes, I will 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 from one box it goes to another box and therefore I can model it very much more easily.

There are other ways to do this. 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 of generation.

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

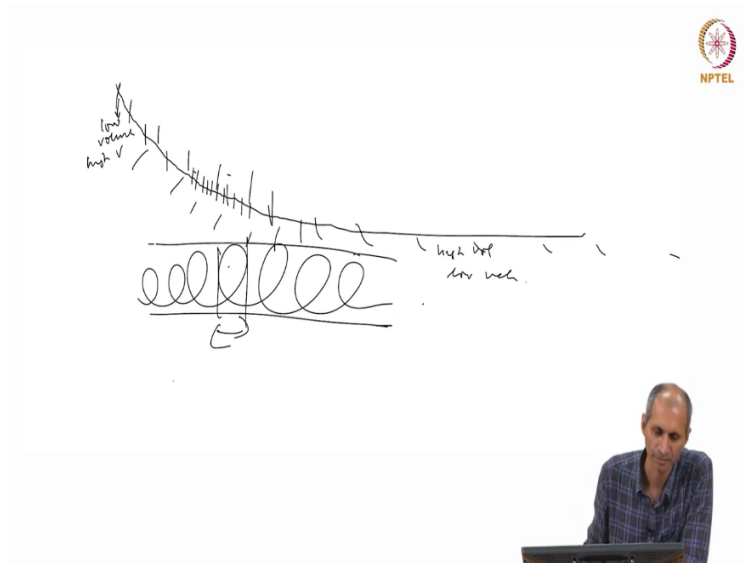
So, here this is my equation so, if I put this in the form of the sink flow, the flow rate of the chemical multiplied by the concentration at inlet equals to what is going out. Now, the unit of this is this  $Q$  is volumetric flow rate, so it is  $L^3$  by  $T$  into  $MA$  by  $L^3$ , this is  $MA$  by  $T$  this will also be the same. Now, if you notice here, this  $\rho A_2$  is the concentration that is leaving the system which is also the  $\rho A_2$  since I am assuming it is well mixed, 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 as an advantage, in the box model in case if I extend a bunch of box models for a series of box models there. I may have  $\rho A_2$  in there entering. And here I may have something  $\rho A_2$  that is exiting the system.

It will also possible for me to model as what is called as a plug flow reactor. I can take small section like, this is flux flow that is going in this direction, the mixing in one zone.

But as this progress from one zone to another zone there is a difference because it is losing material as reaction is happening. So, the reason box model is used in practical systems like the environment is that unlike chemical reaction engineering where blood flow, here 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, the 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. 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 it becomes very different.

The cross section of the river is very different. So, there are a lot of tributaries that join and there are a lot of cities that join. So, it is very difficult to predict the quality of water throughout modeling the entire river as one segment which is later divided into a lot of segments. Now, it is very unrealistic to consider river as a well-mixed system because what we consider as well mixed system it 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. You may have a little bit of back flow because river may flow like this. But scale of



this conviction 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, in order to model these kind of systems. So, if we take the same system, box model. 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, I do not know what is the dimension of it, I have to assume some dimension. So, this is a much trickier problem in atmosphere science but people have to work on this and we will come to that. So, a box model is used like this. So, what we will do initially now, 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 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 we consider them as a steady state except things like lakes.

Where we know that no fluids coming, but lakes also you cannot consider them a steady state in a certain period of time and, 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.