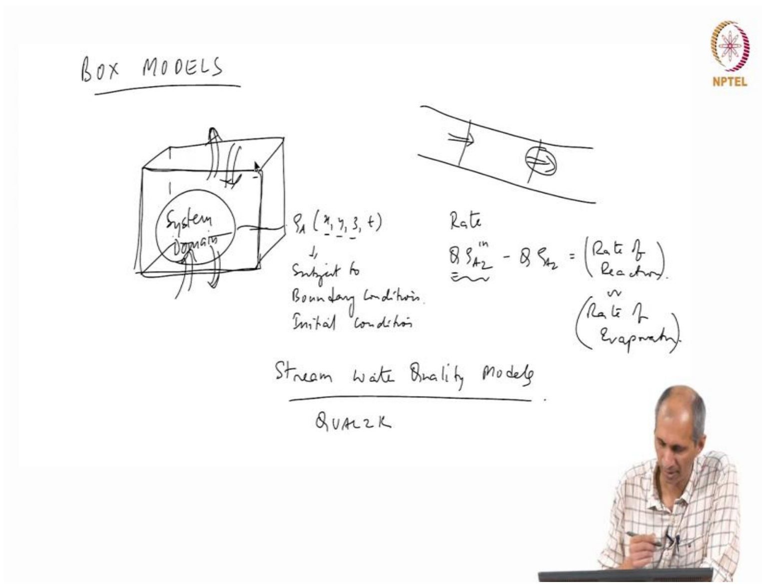
Environmental Quality:
Monitoring and Analysis
Prof. Ravi Krishna
Department of Chemical Engineering
Indian Institute of Technology-Madras

Lecture No. 35
Transport of Pollutants - Box Models in Water

(Refer Slide Time: 00:12)



Okay, so we will continue from what we were discussing last week we were discussing box models. So, the reference to the box model essentially is a convenient way of handling transport of fate and transport of pollutants in a large system. So, in general when you are trying to model a large system, but the general rule of modeling is the following. So, if you have you have to define a system where domain system domain where some processes happening.

So, in the system domain process could be material is moving from one place to other place reactions can be happening material is changing transfer transferring from one phase to another phase within this and then your goal is to find out rho A as a function of as the function of x, y, z and time t this is general objectives subject to whenever you have x, y, z you have this is subject to the boundary conditions and initial conditions this is a general problem definition.

So, in the system domain there is an equation that will describe what is happening in the system? So if there is a rate process or transport anything happens and then there is boundaries of this so, if you look at the system definition for say environmental system water, for example, if you take a lake it is very nice very well defined boundary, we describe that problem because of that has some bond whether it is regular shape or irregular shape it is some boundary.

So, it is possible for us to model it when you have a reverse very large system properties of the system change with x, y, and z. So, system itself system definition itself is changing the function of time for example, if I take a river and we discussed it last class, so, we have rate in - rate out itself. So, we are talking about rate in we use this term Q into rho A2 this Q is flow rate of water that itself may be changing.

Because there may be an inflow of some other stream and then equals say rate of reaction. The rate of reaction is now dependent on few other factors first temperature or perhaps have a third a second compound, or we say rate of evaporation, it depends on the velocity of the water or velocity of air, whatever the conditions of mass transfer, we will get to that later. That is the reason we would not discuss this now, because these terms have to be defined.

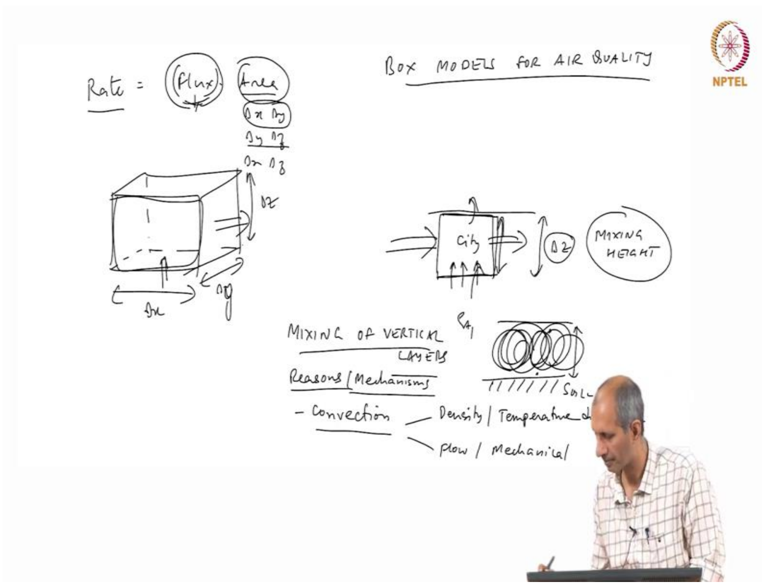
And that requires us to look at interface mass transfer, we will do it in the next section. So this is the movement of chemical within the phase itself requires you to define these terms here. And so these terms can change over a period of time. And that is why we use box models as a convenient way of describing what is happening in a given small region and then extending into the next and so on. So the conditions of one box will become the input conditions to the next and so on.

So, you will have a very large number of boxes it is like solving a set of linear equations. So, you start one point in that one point is the boundary condition you start with something and it is something, you know what is at the end point it does not match you go back and redo it. So, solutions are done like that. So, when you this kind of box model is used for water quality there is there is a set of models.

If you go to the EPA website, stream water quality models, number of water quality models that US EPA has so, each one this one to call this something called is QUAL 2K and QUAL 2E and few other things is on the box model called stream itself various agencies which EPA various people have developed models and EPA adopted them so they used it so in this very important system definitions you need to define the system.

If you are saying I am using a box model, I need to be able to define the system defined dimensions are the system minimum. So, because here the A lot of times what we are doing when we go to transport models, we are transport out of the system or into the system. We are working on a flux based approach you did not work on rate base.

(Refer Slide Time: 05:46)



Because when we say instead of rate, we say the mass balance is written in terms of rate equals flux into area. The reason we do is this is a convenient way of expressing mass transfer or transfer from different places. And when we are doing flux, we need to define the area itself will either mean delta x delta y nor delta y delta z nor delta x delta z any of these 3 things. So, we have a system like this, which is defined we say this is delta x this is delta y and this is delta z.

So, depending on this surface area is delta y delta z this surface is delta x delta y and this surface will be delta y delta z depending on which interface are we using we can we need to add that area. So, therefore, appropriately we need to calculate the flux. So, mass transfer flux in a lot of terms are as mass transfer is estimated in terms of fluxes and it normalizes the area and for good reason we will see that later.

And for the rate involves area which means the rate if you want to write a mass balance equation you need to write the, define the system you need to know the volume on the system on that system. So, delta x delta y delta z should be in this poses a problem in when we go from a river kind of system to air. Air we did not have a physical boundary is air exists in throughout you know, it is an entire expanse of air.

So, if we want to write box models for air quality, it becomes a problem. So, people do the box models for air quality. So what they will do is if I want to look at regional air quality, second the same thing, if I am looking at a particular city and I want to know what is the concentration of some species in air here I am I would like to find out what is coming into the city from somewhere.

And whatever is the sources that are emitting pollutants into this volume above the city and what is being carried out which goes to the next place then and what is being exchanged with the upper atmosphere and so on. So there are all these kind of processes that are happening what is the exchange between the land and air here and what is very critical here the city x and y dimensions of the city are geographical dimensions.

But the z dimension this one, there does not seem to be a very strict boundary for this so if you look at it, you can look at the sky, it seems infinite it keeps going forever. So how will I can I even do a box model for this? Is it reasonable to even approach a box model? It is very complicated system. So there is a reason we see air quality models have a lag period. What quality has been going on for a long time?

Groundwater quality models have also been going on for a long time. Because a slower system is more defined. Only thing is you cannot see groundwater flow, you cannot you did not know where it is, but it is reasonably slow. So you cannot make some assumptions and say that it is here and here and so on. So it is general principles are known the air, it is very difficult to approach this thing. So people have studied a lot in the last few decades and come up with a lot of theory.

And we will look at some of these so, the first problem is, there a vertical boundary to when we consider we want to consider a box model. Otherwise, it is the last case we cannot do any modeling of this nature. So, we have to go to a very, generalized model. So what I mean by generalized model we will see what a generalized model means, which means that you are the full mass balance in its full form.

And then integrated it will become a multi-dimensional partial differential equation in the complicated equation boundary conditions you may not be able to solve. So, we will look at that one of those cases how it turns out. So, it turns out that the vertical delta z people then looked at what is the behavior of this structure of air over the Earth's surface. So, if you want to consider it as a box model then our definition of a box model is everything inside is well mixed.

So, is there a region above the surface of the Earth where you can consider it as well mixed? So, this is not the same kind of concept that we study in liquids for liquid interfaces have this system also but we did not use it in liquids often because the this the thicknesses of liquids are all finite, we know that we can model the entire system, but we have to invoke these kind of principles in air because otherwise we will have no way of estimating air quality.

So there is at least some approach error of some we have something that we can do in order to so, the vertical extent to which you can consider your box model depends on what we call as mixing height. So there are different terminologies to this and some of them may seem contradictory to each other for we will just go over that with something called mixing height, which obviously as the name suggests, this is supposed to be the dimension.

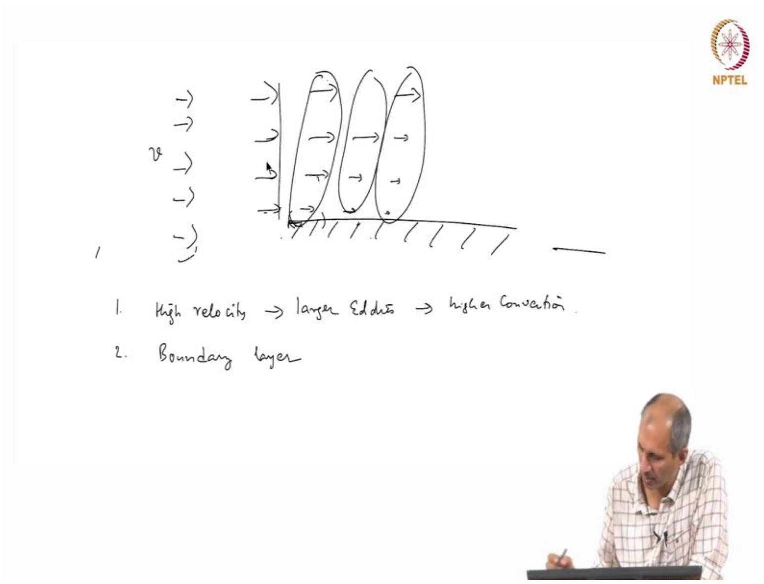
Where your particular extent of box model is some mixing, which means that a pollutant I dropped but the surface will go and mix well into the rest of the mixing height. That mixing height is based on a premise assumption that say this is a ground this is soil. And this is some height here, in which everything is well mixed. Whatever I add here, it is mixed which means that if I measure a concentration of a pollutant here and I measure it here it should be the same that is the assumption that we are making that should be the same.

So, this mixing, so, the next question that comes is how is it mixing? So, you are saying it is mixing, why is it mixing? So, what is the force? What are the forces that will cause it to mix? The first question that we are mixing of vertical layers what are the reasons or what possible mechanisms by which this can happen? What is one mechanism by which this can happen mixing convection, so, one is convection but what is convection?

This convection is a description of the process connections essentially means that you this is happening connection means it is moving in circles. Why is, this moving in circles that is what is the question density difference. Why does density difference out occur? Temperature difference is there another reason for convection flow. So, flow itself is a mechanical energy that is given to the system.

So, it is generally observed that higher the mechanical energy or the energy that kinetic energy that is it has leads to higher degrees of conviction so, we have seen this inflows. So, this is in fluid mechanics theory when you have flow inside.

(Refer Slide Time: 14:11)



So, we have flow normal flow that say you have flow is we have a surface. So, you have flow inside this thing, when you have very low velocity is generally seen that the fluid is moving in a nice element of fluid if I drop a fluid here some element of fluid means if I have a tracer if I can trace the fluid, it is going in nice almost a straight line very close to the surface and far away from it far away from surface it is slightly different.

The reason it is so, is doing something very close. It is the fluid is coming in at very low flow rates. You also have increased the flow rate of this fluid what is observed is that you are seeing this kind of behavior which starts this is velocity v1 as we velocity v2 then v2 is greater than v1, you start seeing some kind of equalization energy tries to distribute itself and it moves this way. And if I go to a another high velocity this distinct start moving in this direction, so, keep on going like this, say I go to v4 and get really large connection.

So, generally the scale of convictions the scale of connection is the distance of this, the size of this these are known as Eddies, the size of the ladies are expected to be larger and larger as velocity increases, velocities or the flow increases. There is one, there is one thing the second thing is very close to a surface. There is a loss of energy. So, if a fluid is coming in with this kind of structure, if it encounters a surface it loses energy and it when it loses energy it velocity drops down.

So, when it loses energy, it is going to assume a lower velocity very close to a surface, then it is in a region very away from a surface. So, for example, you may find that this is very large scale Eddies here, but as you come close to the surface, Eddies may vanish completely and it may assume a very low velocity and as it goes away from the surface as you are away from the surface, it retains its original structure.

So, 2 things here 1 is high velocity generally leads to larger Eddies higher conviction general rule of thumb there are exceptions to this, but there you need other information for this. Second thing is there is what is called as a boundary layer that forms. So what we are talking about in this picture here is that if I draw a velocity profile of so let us say that this there is a, let us not even consider the surface let us say there is just a surface and there is fluid coming in here.

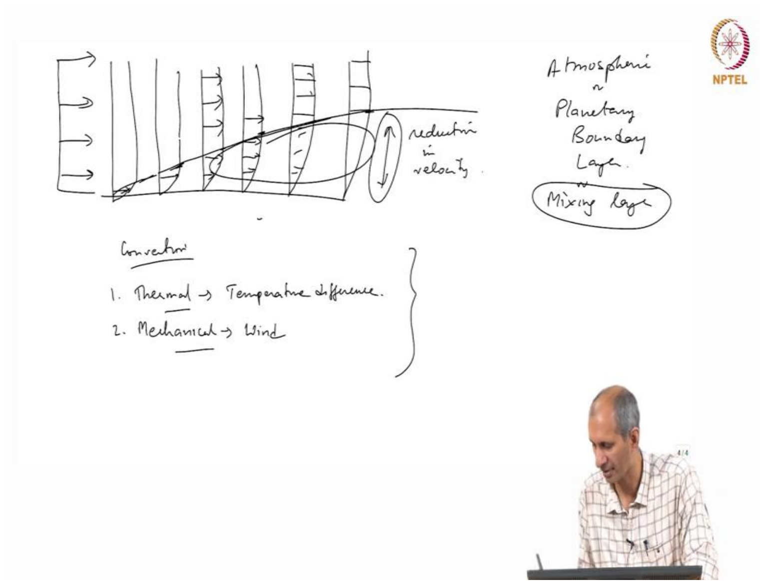
And it is coming in at some average velocity. So it has all let us assume it is uniform, which has large Eddies that are coming in here. The moment it hits the surface. What happens is this, this portion if this is the portion that is coming and hitting here, they are all at the same velocity. But the moment this encounters this land, the land takes up some of the energy just dissipate energy is dissipated there.

And therefore, this reduces the energy of this reduces. And it continues to go, the energy reduction results in a reduction in the velocity. When you say reduction energy essentially translates to reduction in velocity, it is like friction, somebody is running very fast. And as they come to a surface, which does not allow them to go faster, they will float on so it is it is like that is friction in a very simplistic definition, it is friction.

But the regions away from the surface continue in its original state, but this energy in this system is fixed. Therefore, as it moves further down, more energy losses occurring at the surface, and therefore the energy loss has to come from other layers. So when you go that this one slows down even further, this one slow down and this one remains the same. And if we go further even this one is really slows down a bit this one is not here the other one is here like this.

So, it keeps on going for this particular parcel of fluid, the energy per volume is fixed, amount of energy is fixed. So, if it has to pull energy, this friction is withdrawing energy from it from this parcel is energy has to come from the top layers and that results in a reduction in the velocity closer to the surface. So, this results in what we call as a boundary layer as a velocity profile. So, if I plot the velocity profile for this kind of systems.

(Refer Slide Time: 19:42)



If I am plotting the velocity profile here, the velocity profile is flat as it enters there all the same, but the moment it hits it, what we see is the first one this one reduces a little bit, but the rest of them are all the same. But as it goes further and further in, you will see that this reduction increases this curvature increases. So, what we said the region where the original velocity exists is there is a region where if you mark all this point where I am making it straight, what it actually means is in this region, there is a reduction in velocity.

This is what is generally called as a boundary layer in fluid mechanics, this boundary layer is where we assume that the there is a variation in velocity the velocity profile, but in atmospheric sciences this boundary layer exists in nature, it exists because we have surfaces all around the world the entire globe is a surface. So, there is already a boundary layer air is not coming from somewhere else, it is all already there. So, there is a natural boundary layer that exists because there is friction on the surface.

This friction varies from surface to surface. So, if our own natural grass there is a friction on water, well, it is a different kind of friction. If we are on buildings a different kind of friction, sure, and forests have different kind of friction. So, this boundary layer varies that is one between said there is a velocity gradient. We already mentioned that if there is a velocity with the velocity is lower, then it is very unlikely to have very large convection.

So this is where the contradiction comes with the boundary layer, this is boundary layer is the physical definition of the boundary layer of this there is a velocity gradient in the within the boundary layer this is the definition fluid mechanical efficient of boundary layer, but the there is something a term called us atmospheric or a planetary boundary layer. Now, if you look at it this planetary boundary layer sometimes people call it as a mixing layer and all these.

These are not the same kind of definitions is boundary layer essentially is this boundary layer is only layer thickness should not be very high. But there is another boundary layer which they call as a planetary boundary layer where the, that is slightly higher where what they expect is that this entire region is well mixed and that is used to calculate how pollutants move in the region above the surface of it this one is useful in estimating fluxes of chemicals from the some surface to the air.

So, we will come to that later but the other definition that we use is mainly means, what is the mixed layer which is the is there a ceiling to the atmosphere by which you can assume that there is a vertical height or I can assume that vertical height to calculate the concentration of chemical in that layer. So, to get that information there are 2 things are there so, now, we know that the vertical height is a function of the connection that we have and the convection has 2 forces to it.

One is thermal, which is based on temperature difference that we mentioned the second one is mechanical. Since mechanical is mainly the wind velocity, thermal is the temperature the temperature difference. Now, in order to explain this people have come up with a couple of terms. The first term in that context is to find out under what conditions the thermal and mechanical forces how do, they influence the vertical movement of pollutants. So, this is from a pollutant point of view, this these definitions make a lot of sense when you are looking at pollutant behavior, in the region above the surface.