Environmental Quality: Monitoring and Analysis
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Lecture – 50
Estimation of the Mass Transfer Coefficients

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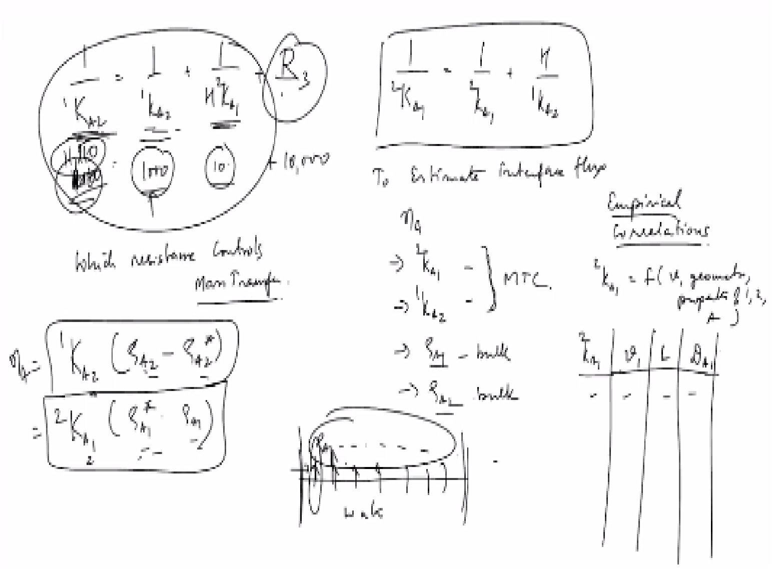

So, one has to get mass transfer coefficient, a measured mass transfer coefficient for different systems and the only a very efficient or practical way of doing it is by using empirical correlations. What does this mean? Empirical correlations means there is we are saying kA12 is a function of several things, is function of velocity, is a function of geometry and properties of 1, 2 and A all of them, a bunch of things okay. The word empirical means that this is a measured mass transfer coefficient under different conditions and we use that in order to estimate flux for a different.

It is very convenient from an engineering point of view. We are trying to estimate it, though we cannot measure it every time in the different system. So, people want some kind of an equation where they can apply and get this done. So, practically, what people have done this they have correlations. Correlations are based on experimental data, yeah. So, you have kA12 experiment velocity with geometry. So what we mean by geometry is let us say that we are looking at mass transfer, the system definition becomes very important.

So it is mass transfer coefficient from lake water, the gas side mass transfer coefficient on a lake. So what does it depend on? We are looking at wind speed mainly first one, this is v1. Then we are looking at the length of the thing. Now, this is a very important concept and if we look at the mass balance that when we did the box model, there is something that, so let us say there is a body of water here and there mass transfer is occurring, yeah. We are assuming this is well mixed, yeah.

We are assuming this is also well mixed, but one of the things that is happening practically is that as mass transfer is occurring, this concentration is changing and we are going across the interface. When we take a small enough section, then the mass balance applies very nicely. There is mass transfer happening, it picks it up and goes to the next section, but if the section is long, there is going to be a difference in the driving force, this number will change, rho A2 - rho A1 star will change, rho A2 star is changing because rho A1 is changing, we are adding material okay.

So the way we estimate this and it will become clear now why we need to do this. This L now becomes an important parameter in this model that L needs to be defined. It is true again with different other mass transfer systems, we will not discuss it right now, but from a more general mass transfer coefficient concept that may be important. We may also have diffusion coefficient of 1 DA in 1. This is important because we also mentioned earlier that the flux mass transfer coefficient is a combination of both convective and diffusion terms.

We do not know exactly which one is dominating. We are assuming it is the velocity that dominates more, but we still have DA and there is likelihood that something with higher diffusion coefficient may have a marginally higher mass transfer coefficient depending on where it is, which velocity and all okay and any other factors that are of importance. So what I have to do is I have to measure the mass transfer coefficient at every set of conditions. I will have different velocities of air and I will have different lengths, I will have different DA1.

What is the meaning of varying DA1 if I am saying I will vary DA1 in different experiments, what is the implication of that? What does it mean? **“Professor – student conversation starts.”** We are changing the material. Changing the component, we are changing A, so different diffusion coefficients. **“Professor – student conversation ends.”** We are doing the same thing with different chemicals to see there is a correlation with the property of the chemical itself, the diffusion coefficient itself. So, if you combine all of this, you will get a correlation.

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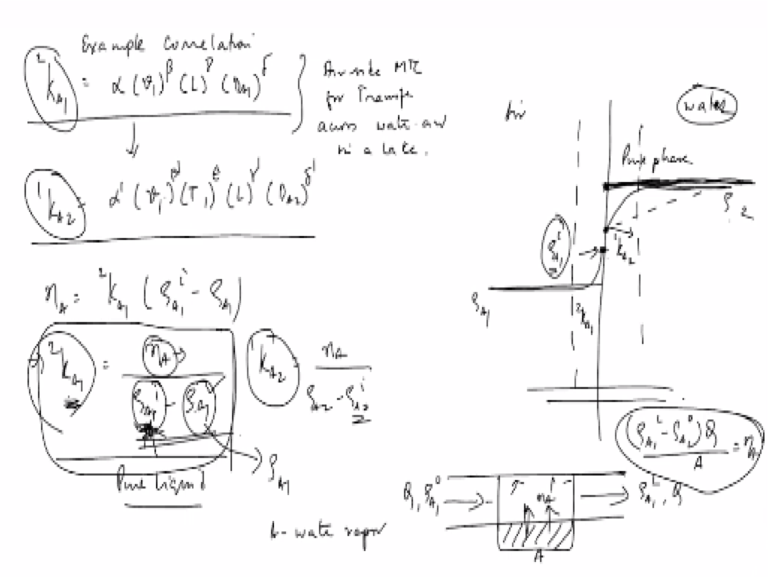

So, the correlation may look like this for example. So correlation may look like this, kA12 which is an example alpha into v1 raised to beta into L raised to gamma into DA1 raised to delta for example. This is a correlation. So, there are some in you will find correlations like this for different systems. So, along with this, people would have also given other conditions. So, this is air side mass transfer coefficient for transfer across water air in a lake.

Similarly, I may have another correlation for the water side coefficient, which may also have alpha bar into v, now the water side part may depend on v2, it can also depend on v1 depending on which whiter there is, so it may eventually, so v2 depends on v1 if there is thermal convection, it may depend on the thermal this thing. So, instead of having v2, we may just have v1 raised to beta this thing we may have some temperature term here raised to we will call it as epsilon L delta DA2, sorry L gamma delta bar.

It may have a different correlation. It will have a different correlation for the water side okay. How do you get this correlation, we said we do experiment, but in an experiment how do you get this? So, you have to use that, the experiment is essentially kA1. If you will notice that to calculate capital K, we need small k and small kA2 and small kA1, but small kA2 and small kA1 are this and to get kA12 is flux divided by rho A1 - rho A1, which means that if I measure the flux and if I know the concentration gradient, I can calculate the mass transfer coefficient.

This is from our basic definition of the flux, okay. However, we have a problem. We have already determined that this is not possible, measurement of this is not possible. So how do we work around this problem? Some of you have taken mass transfer in other courses will know the answer. How do we work around this problem? We have now come back to the same point where we cannot proceed unless we do some adjustment and the adjustment is based on our interface this thing. So this is the kA2, this is kA12 yeah.

Now, to calculate this, we need this, so we are relying on this equation to get our mass transfer coefficient on the liquid side or the gas side whatever the case may be okay or the same equation we can have on this side will be rho A2 by rho A2i. Both of these cases, this is a problem and this is a problem, so how do we work around this? What do we have? So, our options, the clues are on this, on the board here, this diagram. How can we manipulate this diagram so that we measure what we measure and still get an individual mass transfer coefficient. How can we manipulate this diagram?

How do we manipulate this diagram so that whatever we measure here is the mass transfer resistance in one phase, either liquid or gas. So, for example, we take the case of kA12, measurement of kA12. We had this example yesterday, kA12 yesterday yeah, think about it. Very simply, our problem seems to be that I do not know what is rho A1i which under what condition do I know rho A1i? **"Professor – student conversation starts."** Is there any condition under which I know rho A1i? Well mixed.

Well mixed, but we have already started mixing it, it will still give a small region. What is the maximum limit of the well mixed condition? They are still in equilibrium. By saying well mixed we are saying uniform concentration throughout all the way to the interface, is there a condition where this is true? Is there any case where this will be absolutely there is no question that this will not happen. In other words, what we are saying is there any condition by which this becomes a straight line, going all the way to interface? High velocity. Higher rotation or velocity.

Higher velocity, but still there always is a small region. Very slow transfer. This is no, very slow transfer will mean this, this will become more and more, the gradient will be very very slow. Very fast. Any, anything else? **"Professor – student conversation ends"** This is the clue, the straight line goes all the way to the interface, what does this mean? There is no change at all. Yesterday's class we discussed this yeah, at the interface between rho A2i and rho A1i we said it is equilibrium which is Henry’s constant.

But before the Henry’s constant, we said to get you to that point said one special case, what was that remember, to illustrate that at the interface things are in equilibrium, there was one special case we discussed, okay. One of the ways in which this can happen is this entire thing is the same compound, we have pure phase, pure chemical, for example if you have only water, there is no solute. There is no solute, which means there is no A here. There is no A, the A is water yeah, but water at the interface, in interface with air water will evaporate.

This is there is no significance of this concentration of water in water, that is this is density of water that is all, but at the air side, what is this concentration? There is still a rho A1i, what shall that be. This is pure water on this side, what is this concentration? This is saturated vapor pressure, this say one that is in equilibrium with this. So, what we have done we have manipulated the system in such a way that this is true. This rho A1i is known, is measurable because this is pure phase.

Our problem is that we do not know rho A1i, rho A2i in a case where there is a solute because we do not know what is the thickness of this thing, but if you say we do not worry about the solute, we are saying this. We just have one component, it is pure phase, everything is there all the way through and we are tracking that compound coming into the gas phase, air phase. So then the problem becomes easier because this number now you can estimate rho A1i, no? Not convinced?

So, we do the experiment with a pure phase, in pure liquid there is no question, this line has to be straight whatever the value is, it does not make any sense. This concentration is not relevant anymore, but here there is a gradient that exists. So, when you do the experiments like this, this is measurable. So, what will this be? This will be the concentration of water, which is 2, concentration of water, this is A1 where A is water vapor in ambient air and this term will be the saturated vapor pressure of water at that temperature and you can measure the flux, that is now flux measurement becomes very important.

Flux measurement is how much of massed water vapor is evaporating in the system now becomes an important measurement. You know these two by other measurements. So, for example in an experiment which is looking at this, I have water here, I have air going in, say at some concentration, we call it as rho A1 and air is coming out at rho A1L. We use the box model here, simple mass balance and this is coming in at a flow rate Q okay and this is the flux.

So, simply we say rho A1L - rho A10 into Q divided by the area should give me the flux assuming that water vapor is not going and sticking somewhere else, whatever is the change that you are seeing here is exactly what is coming out. Practically, there are problems, things will get stuck, absorbed here and all that, all that is secondary experimental error issues, we will not go there now. So, the measurement of flux experimentally related to the concentration gradient that we can estimate, will give you the estimate of the mass transfer coefficient.

So, we do this kind of experiment for what is the reverse, if I want to look at KA21, what can I do, the same way what can I do? I now assume that, I do the reverse. So, there is one very important thing that you have to understand here.

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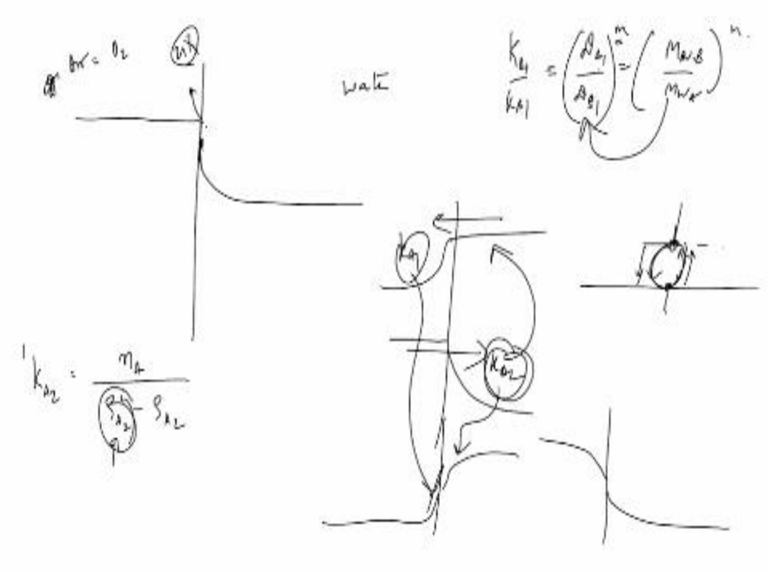

Now, if I want to do a reverse experiment, I will have to now take something that is pure phase here and then air and water. So, what can I do here in this case? So, we are now talking about k21 equals nA by rho A2i – rho A2. In this case, we want a system just like this, just the opposite of the water evaporation, we are using something which there is no gradient, what can you use, like what we used you can use a pure gas okay, but an easy or something which we know the concentration is the same all the way through.

So, once we already have that and ready readily available is air itself. The oxygen in air is, so the concentration is very high and expected to be uniform throughout, that is it is not a solute that you introduce somewhere and go with. The composition of the atmosphere is such that oxygen is not segregated in one pocket of air and all that okay. So it is throughout the same. So the concentration of oxygen and air is known and its solubility inside water is known. So we start with the solubility of oxygen in water and then that is the gradient that we draw.

So it is 21% of oxygen in air that is already known. So correspondingly there is a water concentration that is known and this is what we use in this case. So, we look at mass transfer of a gas into water to get the water side mass transfer coefficient. We look at the evaporation of vapor from a pure vapor to get the air side mass transfer coefficient. You can do any kind of experiment like this. So what we are doing is we are manipulating a system so that we get this.

Professor – student conversation starts.” Sir but that kA is changing no sir. In the first case it was kA, A was water, but here it is oxygen. Yeah, so why does it matter? Good question why will it matter. **“Professor – student conversation ends.”** There is another question that follows this. So, this is important. So, in our previous this thing in this table, we are already seeing that we are measuring this with DA1. So, you do with multiple vapors and check if this is true. You can do this with water oxygen, then you do with some other vapor, then another vapor, and so on.

So, you can have pure gas and we have pure water, we introduced pure gas in an experiment and see, but in the environment this is very difficult to do. So, what we will look at is this correlations, people do not like correlations. Our system of interest is a lake or a river or an ocean. If you do an experiment in a lab, you cannot recreate that. So people are always interested in getting field data. They want to check if, that is why we use oxygen in this thing.

Now, how do you convert a mass transfer coefficient that is measured with water and oxygen to some other vapor, they want to use it for benzene or you know some vapor phase chemical which wants to get in, how do we do that? Relevant question. **“Professor – student**

conversation starts." Dependent, depending upon the molecular weight it can. So we scale it like what we said yesterday. **"Professor – student conversation ends."** So we said yesterday that DA1 by DA2, sorry DA1 by DB1, two things it is scaled by molecular weight of B by molecular weight of A raised to something.

Now, this is a function of kA1 by kB1, the mass transfer coefficient is also related to DA1 by another, so, I will input this relationship into this one. It is all experimental data. So, I calculate mass transfer coefficient for one chemical and another chemical and then see what is the relationship between these two? How does it correlate with molecular weight? So it turns out this is approximately like this. So this n is around 5.4 or some such thing for, vapor and liquid is different, so just the way we are scaling these, we are scaling for this.

So, if you are unable to do an experiment for a wide variety of chemicals, you do for one and then you have to scale it for another one. So, in those conditions, the correlation will have to have if this is not there, one has to specify for water vapor, yeah, which means that you know what to scale with, this is only meant for water vapor. If somebody has done an experiment only with water vapor for a set of velocities, this correlation is only proven for that system. You have to scale it to whatever conditions you have.

If you do not have any other correlations, you have to scale it yeah. There is another question that should follow. When we did the water evaporation, we were looking at a gradient that was this way, and when we were looking at oxygen dissolution, we were looking at a system it just looks like this. The mass transfer we are looking at in this direction and here the mass transfer is in this direction, but I am estimating kA1 using this and I am estimating kA2 using this and then I can take this and apply it to a system where mass transfer is happening like this.

I will take this kA2 and put it here and this kA1 and put it here. Do you have a problem with that? You understand my question? We are disseminating mass transfer coefficient individually in opposite directions and then we are using these individuals to put it in either direction. I can use it in a case like this or I can also use it in a case where it is going like this. The individual coefficients I am using it are applicable in both directions, is that justified? What I mean is if I determine a mass transfer coefficient in one direction, it is applicable in the reverse also.

What do you think? No, why not? In order to invoke what is the definition of the mass transfer coefficient, we are looking at circulation, convection. So, at the interface we are looking at, this is a scale at which this is happening which is convection plus diffusion, irrespective of where which direction the gradient is, this does not care. This is a hydrodynamic or aerodynamic thing. It is going, whether I introduce a chemical from this side or introduce a chemical from this side does not matter.

If I put it from here, it will take it here. If I put it from here, it will take it here. So, the convection is happening from place to place. So, whichever side you feed it from, it will take it to the other side. Diffusion of course depends on the gradient. So if gradient is in this direction, it will go this way. If gradient is in opposite direction, it come this way, so it does not matter. Theoretically, it should not matter for most cases, there may be small exceptions. That is the reason the mass transfer coefficient, individual coefficients are determined by using this kind of system. We will stop here.