Environmental Quality: Monitoring and Analysis
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Lecture – 52
Evaporation from Different Surfaces

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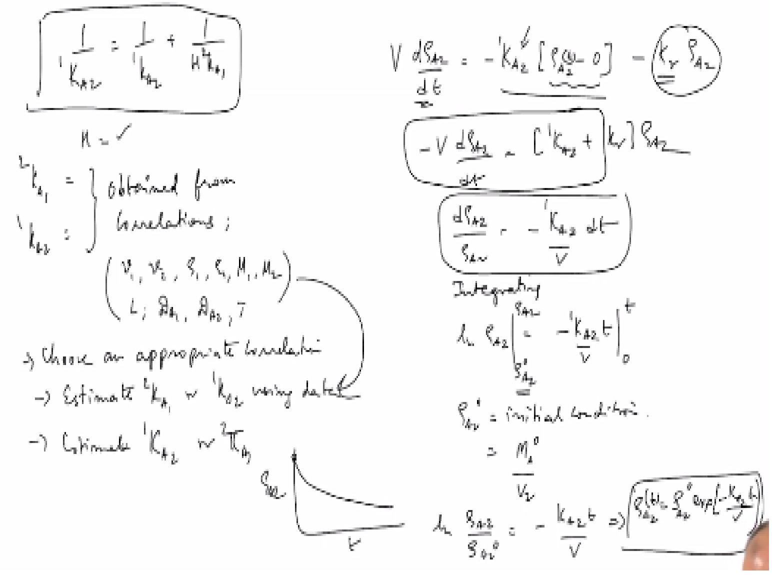


So, we have KA2.

$$\frac{1}{{}^{1}K_{A2}} = \frac{1}{{}^{1}k_{A2}} + \frac{1}{{}^{2}k_{A1}H^{2}}$$

We derived this. So, now, this is the next step. Now, we have the driving force in place we know that, this is the next step. So, this you have to calculate, n is constant it is already known, should be known for the chemical you are looking at. The mass transfer coefficients kA12 and kA21 are to be obtained from correlation. So, there are a variety of correlations that are available in literature. People have measured correlations for different scenarios.

So, you will see there is a sheet in the course page, there is a list of mass transfer coefficients. There is one particular sheet there, it will give you and that is the limited set of coefficients. There is a handbook of chemical mass transport that is available. So, where we have very large series set of mass transfer coefficient correlations for various environmental scenarios, so evaporation from a lake, evaporation from river, evaporation from oceans and all that. So corresponding to whatever is your scenario, so you have to pick the correlation that is appropriate for your problem.

So for a lake, sometimes it will be lake mass transfer coefficient for a lake of a certain length, diameter, certain depth and all that. So these kind of conditions will be there. And to get the correlation data, we saw yesterday that the correlations are usually of the form where you have different velocity of water, velocity of air and water and the properties of these things, density of water, density of air, viscosity of air, viscosity of water, so on and length, diffusion coefficient of A in air and A in water

These are all some of the parameters that may be involved in this thing. So, there is enough information that you need and temperature may be needed sometimes in order to get this. So, this is to get the correlation, that is the first step and choose the correct correlation, and you estimate kA using the data that is given to you, using the environmental data. What we are talking about using all this data. All this data go into this to compute, so just plugging in the numbers, you will get some value, that is all, there is nothing else to it.

You get this numbers, put it in there and calculate value. Once you do that, you go back to the calculate, estimate ${}^{2}KA_{1}$ or ${}^{1}KA_{2}$, the overall coefficient. Now we go back to the main equation, our first problem. So we have now

$$V\frac{d\rho_{A2}}{dt} = -{}^{1}K_{A2}\left(\rho_{A2}^{(t)} - 0\right)$$

This becomes our problem now. This is our differential equation, we know this term now, we have estimated this term, this is a function of time. Because this is changing, this is a finite problem, so it will change.

So this is minus here because it is the second time in the mass balance. So, the convention is generally, this is a positive term, this entire thing is positive, this is a negative term because since the system is losing A, the concentration of A in a system will decrease. So the convention is to write all terms as positive. So, it is generally written as this

$$-V\frac{d\rho_{A2}}{dt} = {}^{1}K_{A2} * \rho_{A2}^{(t)}$$

$\rho_{A2}^{(t)}$ is a function of time. So, here we rewrite this as

$$\frac{d\rho_{A2}}{\rho_{A2}^{(t)}} = -\frac{{}^{1}K_{A2}}{V}dt$$

very simple equation.

We integrate this, we have

$$\ln\rho_{A2} = -\frac{{}^{1}K_{A2}t}{V} + c1$$

something like this or alternatively, this is one way of doing it. Alternatively, what we do is we do an integration, we start from time t = 0 to some arbitrary time t, this is rho A20 to rho A2. The integration will be finite integration limit. So this rho A20 is now the initial condition. So, this is the first order equation in time, so initial condition is required. So, this initial condition as you are pointing out is now initial condition of this has to be determined.

So you say finite amount of chemical was dumped into the volume. Say if M_A^0 was dumped into the volume, this divided by the volume of lake should be the initial concentration or by any other calculations, by equilibrium calculation or some such thing which we discussed in the beginning of this course can also be used, any number can be used here. So as long as you know what is the starting point of that, okay. So this equation will be

$$\ln\frac{\rho_{A2}}{{\rho_{A2}}^{0}} = -\frac{{}^{1}K_{A2}t}{V}$$

, essentially this becomes

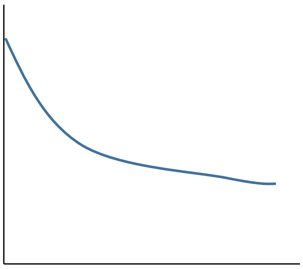
$$\rho_{A2} = {\rho_{A2}}^{0}.exp\left(-\frac{{}^{1}K_{A2}t}{V}\right)$$

This is a very simple, this is like a reaction, first order reaction. This is like a first order reaction equation. So, we have this term here or this term here, we are seeing that the rate is the first order term, evaporation is the first order of term. So when we say convective mass transfer, it is a first order process. It is like a reaction. I can add other terms to this. I can add another reaction term here, which is also a function of the temperature of this thing. If I do that, sometimes this happens when biodegradation is taking place in a system.

So, you have some reaction that is taking place, it is a first order reaction, and so this entire term now will become

$$-V\frac{d\rho_{A2}}{dt} = ({}^{1}K_{A2} + K_r)\rho_{A2}$$

Each of these terms have to be determined separately. This is an addition, so usually, but this information is only available if you already know that biodegradation is possible in the system okay. So, you solve this. So, based on this equation, I can find out rho A2 at any time as a function of. So, if I plot this equation, I will get something like this, is an exponential.



So rho A2 as a function of time it will start at rho A20 and it will go. What can I do with this information? I am calculating concentration versus time, what is it useful for? To use this in any other kind of scenarios that from an environmental perspective.

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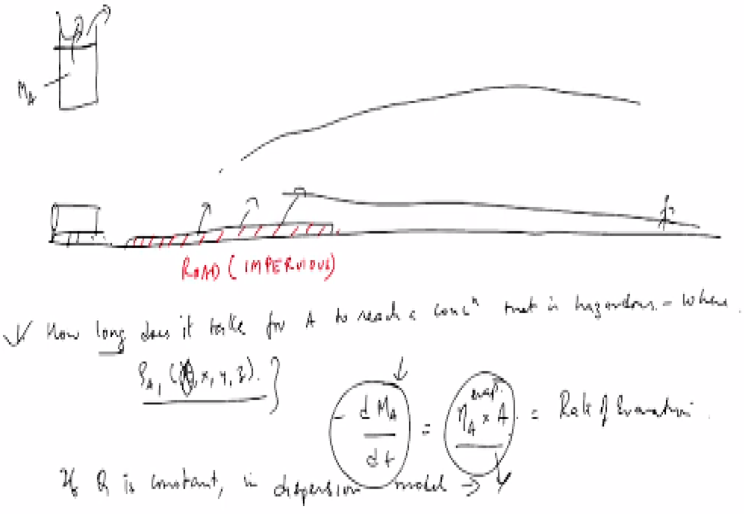

✓ How long does it take for A to reach a concⁿ that is hazardous - where.

$\rho_{A_1}(t, x, y, z)$

$$-\frac{dM_A}{dt} = \overset{evap}{\eta_A \times A} = \text{Rate of Evaporation}$$

If Q is constant, in dispersion model → Y

Suppose there is a big spill in a lake, somebody has, there was an accident. A lot of material has fallen down into a lake. Let us take a simpler case okay. Let me take a simpler case. Let us say we are traveling on a road okay? There is a big tanker that is carrying say 1000 liters of chemical. All this chemical is spilt now onto road. We have a chemical sitting on the road. This is this road. We will consider this road for the time being as impervious for obvious reasons. Problem becomes very simple if it is impervious okay.

Now, what is your main concern here? What is the problem that you will pose now? So, in the previous problem, what is the question that we asked? The previous problem if you look back at the first part of the problem, what is, this is the definition of the problem. I am asking this question what happens to A in the lake? So, which means if my concern there is what is the concentration of A in the lake as a function of time, why am I worried about that? What are the possible reasons I am worried about that?

Student: Maybe how much time it takes to,
Professor: yeah, but why? Why will I worry about how much A is there in the lake?
Student: We are using that water for some use.
Professor: You are using it for something. You are drinking that water or there is fish in the water, animals in the water, and you are going to see what is the risk that is posed to them? Whether you should do anything? Should evacuate all the fish, take them off somewhere else until this will do something, until all of this evaporates. The flip side of the problem, what is the other side of the problem? It is another pose.

Can you pose this problem differently, and that is why I have given this example. What is the example here? What will you look for here?
Student: Risk to humans.
Professor: How?
Student: It is getting into air.
Professor: It is getting into air, so what is the question that you will ask?
Student: Volatile or not.
Professor: Can you be more specific? What will be the exact question that you can ask? It is evaporating, that is the only thing. We have said that the road is impervious and then what is the only way in which it can get to?

If we say the road is pervious, then the question will, if it is soil for example, if it dumps on soil, the question will be, will it get into soil? Will it reach groundwater? How long will it take to reach groundwater? So in this case, we have removed that because that is a second problem, that is a different problem. So, this is like this, what is the question you will ask? What is the design question? This is a design question. It is a question that we will ask in order to do further things. The question that you can ask in this problem is?

Student: How long it takes to reach the minimum concentration?

Professor: Where?

Student: In air.

Professor: In air, where? This problem has been posed like that so it is where? Your question is how long does it take for A to reach a concentration that is hazardous, this is incomplete. You are talking about how long, but the next question will be, where is it? Where?

So, essentially we are asking rho A1 as a function of time and space. What is this problem now? What kind of problem is this? Do you know how to calculate this? What kind of problem this is? How will it reach a particular receptor somewhere down wind. By what?

Student: Air and wind.

Professor: What is it called? We just did this last week, by dispersion. So, this is a source. So it is getting out and it gets carried down wind. We would like to know what is the concentration? So is it a steady state problem or unsteady state problem?

Unsteady state. Why?

Student: Because time is involved and it will never.

Professor: How will you decide if it is steady state or unsteady state? Essentially what determines that? This is a difficult question to answer. We are asking this question because now it will help us model this system. So, if I want to answer this question, whatever I have asked here, dispersion model, is it enough, sufficient? So here in this question, I have a t here, yeah. This t, if steady state model, t should not matter, it should be the same.

It only distance, location from the source this matters. So the next question I am asking is let us say if I am assuming t is not a factor, under what conditions will t not be a factor? The amount of chemical is not changing on the road, but that is not true, right. If I take the same problem and pose it in the previous problem, what will be the mass balance? The mass balance will be

$$-\frac{dM_A}{dt} = n_A \times A = rate\ of\ evaporation$$

this is the rate of evaporation, that is all.

It is evaporating and if x amount of mass goes out, this is changing, but will that change the flux? For a dispersion model, you can assume steady state as long as the Q, the flux or area of the Q term is constant. If Q is constant in the dispersion model, I can assume a steady state model, under what conditions will Q be constant, M can be changing, will Q be constant here? Q is the rate of evaporation, written down here, rate of evaporation is this, this into this.

Can this still be happening, but then the Q, this is true, but from a dispersion point of view, can this still be happening, can this still be constant? How can the area? Let me give you a different problem. I have a beaker of a chemical okay. Let me say that this beaker of chemical has some amount of mass always there and is evaporating. The area of evaporation is always the same. What about the flux? So, let us start, let me redraw this problem.

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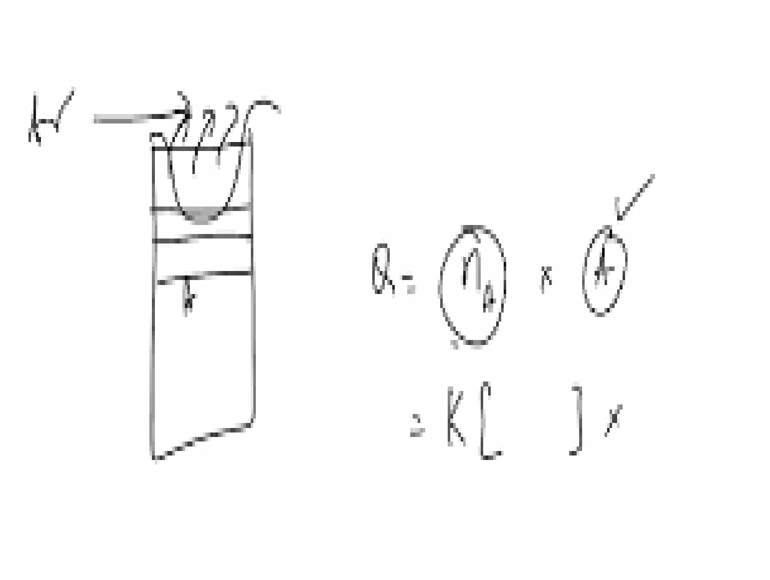

So I am starting with a beaker full of some chemical, some A, pure A, let not worry about solution and all that, pure A. There is air passing over it. As evaporation is occurring, will the rate of evaporation remain the same? What is changing? So we have

$$Q = n_A * A$$

which of these two will change?

Student: nA.

Professor: nA, why?

Student: Because the driving force will change.

Professor: Why will driving force change? This is K times, 2 terms here, yeah. Concentration of A in the solution and concentration of A in air, yeah. But anyway, you are right. So, this flux will change if this is changing, but not for the reasons you are saying. The concentration will not, driving force will not change, but this will change. The level keeps going down and down, and therefore mass transfer coefficient will change because one of these terms will now be diffusion so that is not, but what is important here in our previous problem is if you assume the area to be the same. So, if you have a spill on a ground, let us assume that if the initial volume of the spill is this much, and then the spill continues to reduce in height like this.

It is reasonable for us to assume that the flux is not changing a whole lot, is still the same. Driving force definitely does not change because it is the same solution. We are talking about pure chemical, not a solution, pure chemical okay. This is pure chemical, okay. So as long as the area, we can assume the area is constant, this will not change. The area is sometimes not constant, for example, if I put a drop of liquid on this, it will initially occupy. It will occupy this big area and its shape will not be rectangular like this.

And over a period of time, what will happen is it will shrink like this, but that depends on the interfacial properties of the chemical. It may shrink more depth wise rather than sideways. So, the area may not change very significantly, it maybe more or less the same, but the bulge will be more and you can assume to some extent the area to be constant. Flux is however constant. What is the flux in this case? What is the flux?

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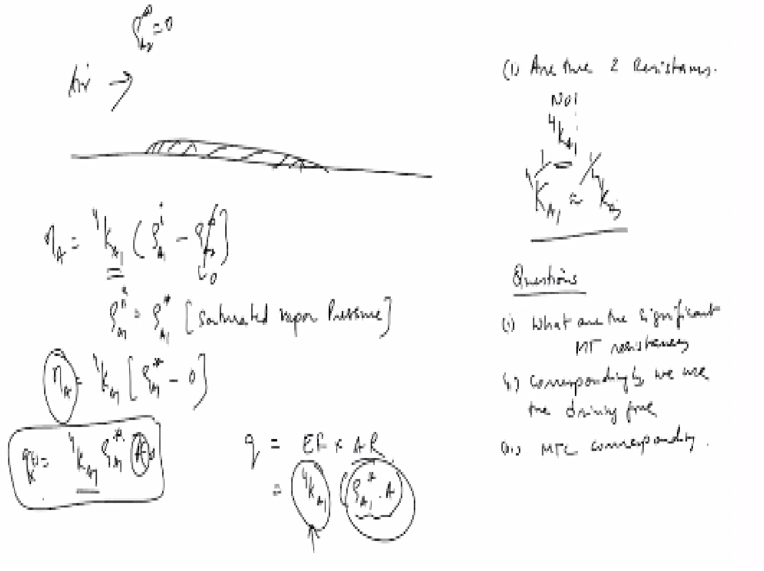

We have pure chemical sitting at some geometry, what is the flux? We need two terms, what is driving force? You have to apply the same procedure, ask 3 or 4 questions. The first question is that are there two resistances? How many resistances in this problem?
Student: One phase.
Professor: One phase, which phase is the resistance? Air. Air, whatever resistance in the fluid? Pure liquid, no resistance. So, answer is no.

So, only resistance we are talking about is $^{4}KA_{1}$ it is pure chemical in contact with this. So, if you are writing this, then it becomes, we have to write this. If you are writing this, then what we are saying essentially is capital $^{4}KA_{1}$ is the same as small $^{4}kA_{1}$. This is what we are essentially writing when we are saying negligible resistance in the other phase okay or 1 over, rather 1 over this, we are doing 1 over capital K is same as 1 over k, which means capital K same as small k.

So, here, what will this term be? There is some background concentration here. This term will be an interface concentration $^{i}kA_{1}$, what is $^{i}kA_{1}$? You know this value, so, this assumed to be 0. What is $\rho_{A1}{}^{i}$? It is Henry's constant. What is $\rho_{A1}{}^{i}$? It is a concentration in the air in contact with pure substance at the interface. What is that? It is an equilibrium with the interface. So, in this case we are talking about concentration of air in contact with pure substance, it is the saturated vapor pressure.

So, the nA becomes

$$={}^{4}K_{A1}(\rho_{A1}{}^{*}-0)$$

This term that you get nA.

$$q={}^{4}K_{A1}\rho_{A1}{}^{*}A$$

This number used to be used as the emission rate. The emission rate for this dispersion problem we are going to solve now and this is a steady state dispersion problem as long as you can assume the A or the mass transfer coefficient to be fairly constant, for that region you can do that okay. The moment the area is changing, you have to change your q value.

If area is a function of time, q will also become a function of time, but the dispersion model is not set up to do unsteady state problem. So, you have to break it up into small times. It will say from first half an hour area this much or average area this much, next half an hour area this much and so on. So you can do the calculation for that one set and then estimate what is going to happen that way we can do.

So here, this is something that we have not seen in the dispersion model discussion, right. Normally when we are doing dispersion,

$$q = emission\ factor(EF) * activity\ rate(AR)$$

right. Here, what is the equivalent of an emission factor? This is not like a point source where somebody is pushing out some this thing. This is a model, a mathematical evaporation model or the dissolution model where a mass transfer coefficient is involved okay. So, equivalence of the emission factor and activity rates, emission factor is the mass transfer coefficient, the activity rate will be the other.

$$q = EF * AR$$

$$q = {}^{4}K_{A1}\overbrace{(\rho_{A1}{}^{*}A)}$$

This mass transfer coefficient does not change, it does not care whether the concentration of whatever is inside is pure phase or a solution, the air side mass transfer quotient is the same, but the activity is changing. This is the activity. The concentration is different, the pure phase concentration or solution. Solution phase comes in, then of course this becomes capital K and all that, that changes. So, we do not call it an emission factor, but other in terms of what controls and what does not usually change with whatever is here.

The mass transfer coefficient whether it is an overall or an individual mass transfer coefficient is now the equivalent of the emission factor for these kind of problems, where it is not a specific fixed source and it is dependent on wind speed and other environmental parameters. So, there are a few questions you would have asked the same thing. So, whenever we do this, we follow the same procedure, ask a bunch of questions as to what are the resistances and then based on what resistance you take we will ask this question of and correspondingly we take the driving force and the MTC.

A lot of times, the biggest challenge is to select the correlation for the mass transfer coefficient because you will not find an exact correlation for whatever you are looking for. You have to find an equivalent correlation which is the closest. So, these are all estimates. There are so many assumptions in these kind of studies, the more complicated studies, you will take longer to solve it and so many of these things are what comes under emergency response.

Suppose there is a spill, how quickly can you tell people that concentration is going to be this much at a distance of 5 kilometers or 2 kilometers. This is a dynamic problem right. On a certain day in a given particular location, you have to figure out so many things, so what is the quickest solution you can give, it is a worst case scenario, and you can use all these assumptions for the worst case scenario, okay? What is the worst case scenario in this?

When you are calculating a dispersion problem, the worst case scenario will occur when?
Student: everything is going to air,
Professor: when everything is going to air, which means q is the highest possible number. The q is the highest possible number that is one. Second is if you are talking about exposure where the wind speed, stability, class and all that you see the most stable, unstable you do not have to worry, it will go, it will disperse fast, but the stable, that is the worst case scenario. If you do not know anything about wind speed, you say okay I assume it is stable and then calculate what is it, okay.

It is over solving, it is over designing, but from a environmental point of view, it is always the safe thing to do. It is okay to be better to be safe than to be, no, after that, this big disaster, that is a problem. So when people design these things, they are working at different scenarios. What if you have a spill on land? What if you have a spill on water? What if you have a spill on concrete? You have a spill in the lab, for example, you are working in the lab, there is quick response, nobody knows what to do.

So there are consultancy companies which do this. They have hundreds of scenarios. They will work on the scenario and then anything happens, they will quickly say this has happened, quickly they have a solution, they already have a solution in place, what should be done. So you can use this to design emergency response systems. The mathematical models are useful in designing emergency response systems. So all you need to know is how much was spilt and what, that information quickly they can come and say 1000 gallons appropriately were spilled.

So you assume it is 1000 gallons or 1000 liters. Maybe all of it has not spilled, maybe something is sitting under something. So you assume the highest area, highest this thing, everything. This is the worst case scenario responses people use it for emergency response. So, whenever we do, so instead of doing post-accident review, these are all pre, so lot of companies have environmental health services, they will do the scenarios. What happens if an accident of this nature can happen.

They will say this is what needs to be done, this is emergency response procedure and if the safety equipment needs to be used and what are those recommendations and so on. So, this can be used in that direction okay. So, we will continue this with more examples next week, Tuesday, Wednesday.