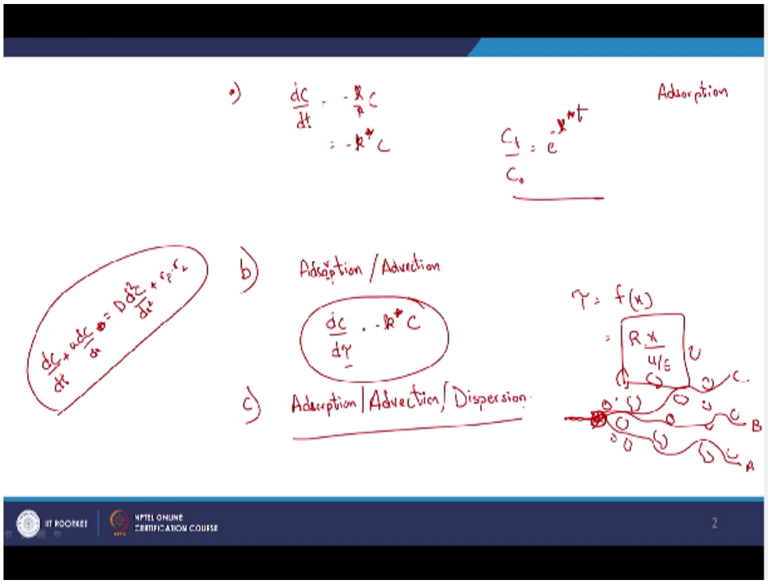
Environmental Remediation of Contaminated Sites
Prof. Bhanu Prakash Vellanki
Department of Civil Engineering
Indian Institute of Technology - Roorkee

Lecture – 28
Rate of Degradation of Contaminant when both Diffusion and Advection are Considered

Hello everyone. Again welcome back to the latest lecture session. Again as is usual a quick recap of what we have been up to. So in the context of remediating contaminated ground water, we are also looking at natural attenuation, right. And that context, we looked at, let us say, how do we estimate, let us say, the relevant parameters or estimate or understand if microbial activity is taking place or not, right.

So in that context, we looked at 2 aspects until now. First aspect, we took the sample from the relevant subsurface, right, aquifer media. And then brought in, conducted the relevant or spiked the relevant aquifer media with relevant concentrations of the contaminant, observed the change in concentration with time and then fit the relevant model. And what was the relevant model?

(Refer Slide Time: 01:11)



So I think we calculated by different ways dc/dt=-k/R or k--C, right, -k--C, right. So from this, what do we have? We have Ct/C0=e to the power of -k--t. So we can fit this model to the relevant particular batch reacted data, right. This is something we looked at. But what do we consider here? Obviously we only considered microbial activity and adsorption and desorption, right.

And second case though we looked at actual data taken along the flow lines in the field, right. So what does that mean? We are looking at microbial activity. We were looking at adsorption, desorption and advection. Advection why is, how is the contaminant being transported here? You have the ground water that is carrying the relevant particular or transporting the particular contaminant when it is flowing in its direction, let us say, right.

So we are looking at microbial activity, adsorption, desorption from the soil into the ground water or from the ground water into the soil and finally advection too. Again we fit the relevant model and so on and so forth. We came up with I think something like dc/d tau=, similarly -k*C, right. So similarly, let us say, we have again what was tau? I think tau was some function of x, right.

So what does this in effect tell you? It tells you how dc is changing with or concentration is changing with distance, right. So that is something that we looked at. What was tau? If I am not wrong, so I think it was x/u/epsilon, I think, this was what I believe we looked at, right. Anyhow, so let us move on, right. I think this is what we looked at. Again adsorption and advection and this is the model and we can fit this to the relevant data from the field and get the relevant constant, let us say.

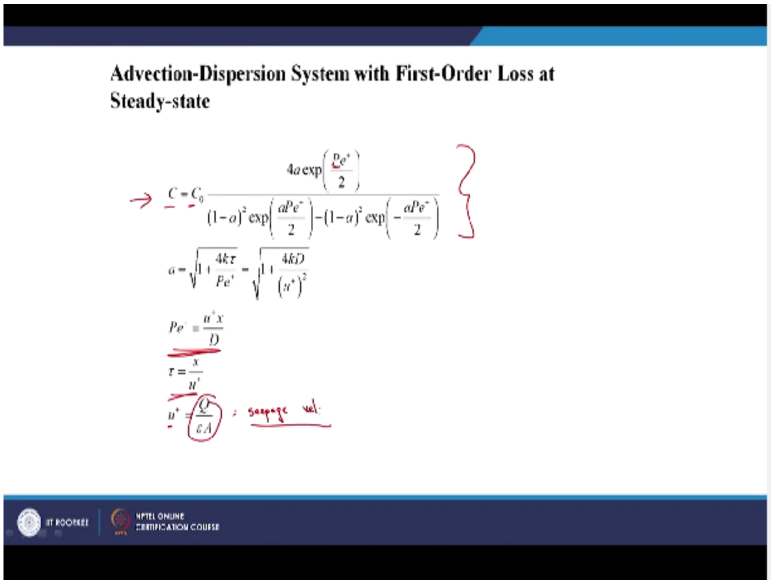
But what are we missing here? Or what is the another aspect that we can consider? We can also consider obviously adsorption, microbial activity and advection, right. But as you know and ground water you are going to have diffusion or more particularly dispersion, let us say. So what is this dispersion now? I think we looked at this value. Let us say, if a particular, this is one particular flow path of the ground water.

And, let us say, contaminant is at this position and you know that this is soil particles, right. So there are many soil particles. So, let us say, this contaminant that comes in here, can take this path and appear this path and appear, this path and appear and so on. So the contaminant that starts at the same location can end up at different locations now, right. So obviously now you see that the concentration is decreasing, right.

Why is that? Because of dispersion, right. Again diffusion and dispersion, we are taking that into account in the same aspect here, let us say, right. So obviously that can be taken into account and looked at. But again what was the fundamental equation we typically looked at? Dc/dt+udc/dx+, if we had the diffusion term, right. That is going to be equal to D second derivative of c with respect to x, right, + or -, rate of formation and rate of loss, right.

So applying this particular equation here or mass balance here and solving for it and such as you see, it is a second order differential equation, right. Which we are not going to go through now but the other people, the others have certainly looked at that. So we are going to look at that particular equation.

(Refer Slide Time: 04:53)



Advection-Dispersion System with First-Order Loss at Steady-state

$$\rightarrow \quad C = C_0 \frac{4a\exp\left(\frac{Pe^*}{2}\right)}{(1-a)^2\exp\left(\frac{aPe^*}{2}\right)-(1-a)^2\exp\left(-\frac{aPe^*}{2}\right)}$$

$$a = \sqrt{1+\frac{4k\tau}{Pe^*}} = \sqrt{1+\frac{4kD}{(u^*)^2}}$$

$$Pe^* = \frac{u^* x}{D}$$

$$\tau = \frac{x}{u^*}$$

$$u^* = \boxed{\frac{Q}{\varepsilon A}} : \text{seepage vel.}$$

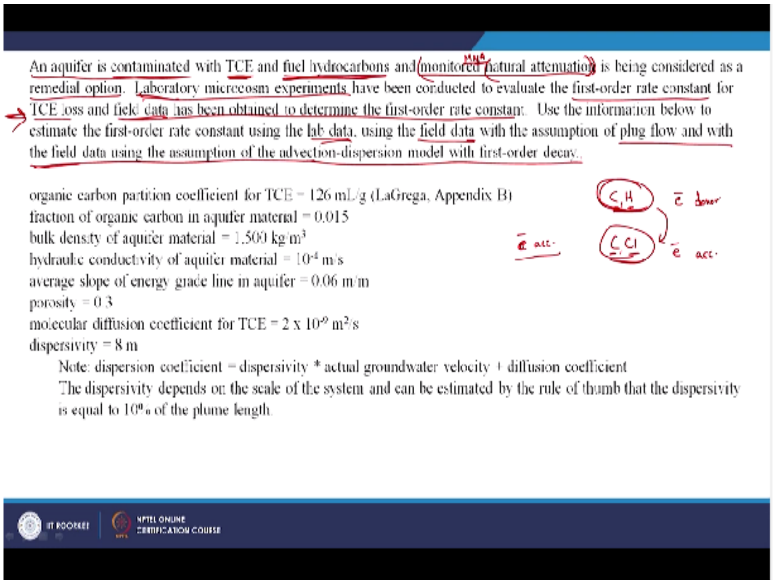
So looks like we can calculate C in terms of C0*, different variables here. P is the Peclet number that is what you have here, right. And what else do we have? We have tau here and we have here u* seems to be seepage velocity, seepage or velocity or the actual ground water flow velocity through the particular pores, right. Again Darcy's velocity gives you the normalized ground water flow as in the ground water flow which is q, right.

That you can easily measure and then the cross-section area of that particular, what do we say, aquifer that you are looking at, you can measure. And Q/A will give the Darcy's velocity. But, let us say, if you want to know the actual velocity of the ground water through the pores, obviously you need to take into account the relevant relatively less area that it has to travel through, right. So thus obviously the velocity will be higher or the seepage velocity will be higher than your Darcy's velocity.

So based on and the A seems to be a constant, right and based on these aspects, you can model C in terms of, let us say, what is it ultimately. C in terms of x, right. This is nothing but C as C0*function of x, right. So that is the typical variable here, right. So again you can fit this model to that particular data and so on and so forth and get the relevant, what do we say, equations, not equations, constants, then understand the system better, right.

Again what is it that we are trying to do? Either we want to predict the relevant rate constants and see how fast the reaction can take place. Or is natural attenuation fast enough such that it can be considered a viable option, right. That is something that we are looking at here, yes. So again moving on now we will look at a particular example and I will try to solve that here, right. So, let us see, what we have here.

(Refer Slide Time: 06:40)



An aquifer is contaminated with TCE and fuel hydrocarbons and monitored natural attenuation is being considered as a remedial option. Laboratory microcosm experiments have been conducted to evaluate the first-order rate constant for TCE loss and field data has been obtained to determine the first-order rate constant. Use the information below to estimate the first-order rate constant using the lab data, using the field data with the assumption of plug flow and with the field data using the assumption of the advection-dispersion model with first-order decay.

organic carbon partition coefficient for TCE = 126 mL/g (LaGrega, Appendix B)
fraction of organic carbon in aquifer material = 0.015
bulk density of aquifer material = 1,500 kg/m³
hydraulic conductivity of aquifer material = 10^{-4} m/s
average slope of energy grade line in aquifer = 0.06 m/m
porosity = 0.3
molecular diffusion coefficient for TCE = 2 x 10^{-9} m²/s
dispersivity = 8 m

Note: dispersion coefficient = dispersivity * actual groundwater velocity + diffusion coefficient
The dispersivity depends on the scale of the system and can be estimated by the rule of thumb that the dispersivity is equal to 10% of the plume length.

So we have, let us try to understand the question here. So an aquifer is obviously contaminated. And what is it contaminated with? TCE, right, tetrachloroethene I believe, right. And here it is a chlorinated solvent, right. And it also has fuel hydrocarbons, okay. So the key here is you have C, H and C with Cl, let us say, right. And typically as you can see which compound is more oxidized and which one is more reduced.

Obviously Cl, more electronegative, it will pull the electrons towards itself. So the carbon in this case will be more oxidized, right. So this is the oxidized compound. H relatively less electronegative or carbon is more electronegative than H, so the relevant electrons will be pulled by carbon towards itself. So here carbon is more reduced form, right. So what can happen here? This can act as an electron acceptor and this can act as an electron donor, right.

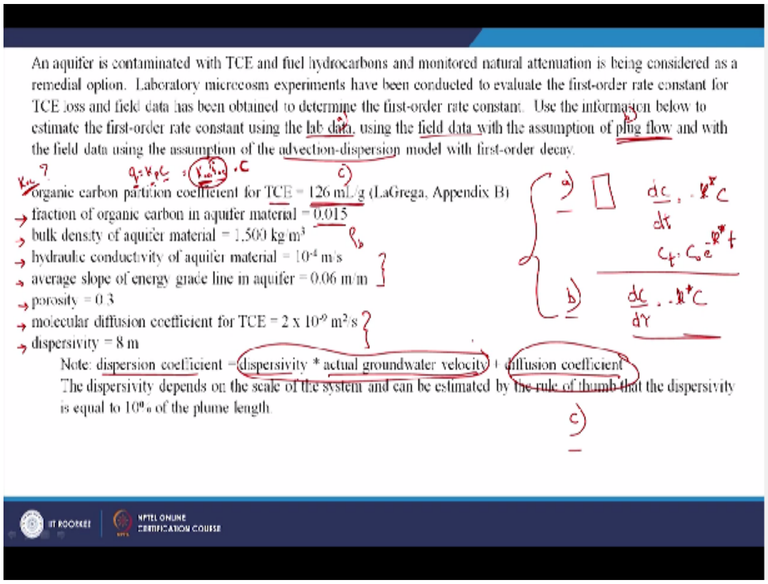
So the electron can transfer from here to here and you can have the relevant reaction and degradation. Obviously this will only take place when there is not other competiting electron acceptable and I think we have discussed this in great detail earlier. But again why is it that no other electron accepted needs to be present here because delta g or the energy that the microbes get form facilitating this reaction to go through, will be relatively less les compared to, let us say, if they have any other electron acceptable oxygen nitrate or I think we looked at sulphate and so on, right.

Any such electron acceptance, they will give more energy to the microbes. So if you have these competing or those competing electron acceptance, then microbes would want to facilitate that particular reaction. Again that is something we looked at. So an aquifer is contaminated with TCE and fuel hydrocarbons, okay. And natural attenuation is being considered as remedial option, right, typically MNA as this called, obviously I discussed it in terms of natural attenuation here.

So monitored natural attenuation is, I believe, legally viable or pursuable option if I may call that in the US anyway, right. Again monitored natural attenuation is being considered as a remedial option, okay. So the first aspect is the microcosm experiments have been conducted to evaluate the first order rate constant for TCE loss. So here we are looking at TCE loss primarily. And field data has been obtained to determine the first order rate constant.

So we have both the laboratory experiments and the field data, okay. So using the information below estimate the first order rate constant using first the lab data, then the field data, one with assumption of plug flow and with the second one being or the second case being field data with the assumption of advection dispersion model with first order decay, okay. So there are 3 aspects here. What are they?

(Refer Slide Time: 09:34)



An aquifer is contaminated with TCE and fuel hydrocarbons and monitored natural attenuation is being considered as a remedial option. Laboratory microcosm experiments have been conducted to evaluate the first-order rate constant for TCE loss and field data has been obtained to determine the first-order rate constant. Use the information below to estimate the first-order rate constant using the lab data, using the field data with the assumption of plug flow and with the field data using the assumption of the advection-dispersion model with first-order decay.

K_{oc} ? $q = K_p C = (K_{oc} f_{oc}) \cdot C$

→ organic carbon partition coefficient for TCE = 126 mL/g (LaGrega, Appendix B)
→ fraction of organic carbon in aquifer material = 0.015
→ bulk density of aquifer material = 1,500 kg/m^3 ρ_b
→ hydraulic conductivity of aquifer material = 10^{-4} m/s
→ average slope of energy grade line in aquifer = 0.06 m/m
→ porosity = 0.3
→ molecular diffusion coefficient for TCE = 2 x 10^{-9} m^2/s ?
→ dispersivity = 8 m

Note: dispersion coefficient = dispersivity * actual groundwater velocity + diffusion coefficient
The dispersivity depends on the scale of the system and can be estimated by the rule of thumb that the dispersivity is equal to 10% of the plume length.

a) $\frac{dc}{dt} = -k^* C$

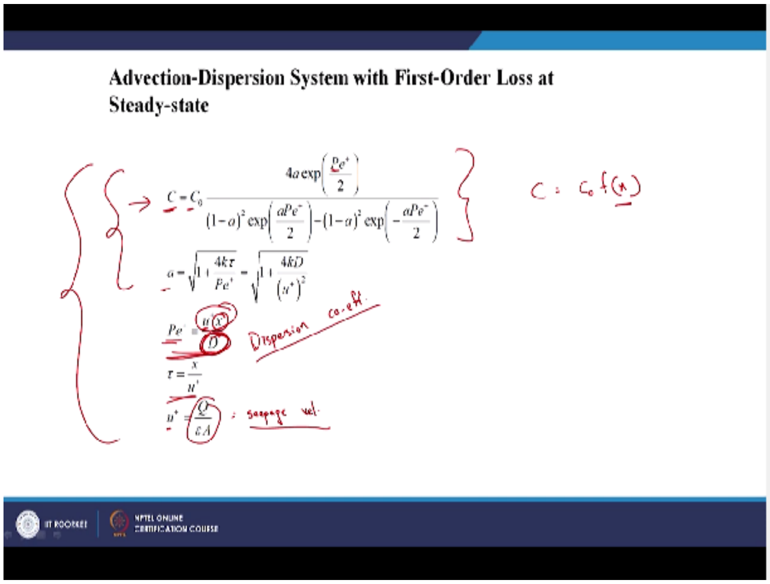
$C_t = C_0 e^{-k^* t}$

b) $\frac{dc}{d\tau} = -k^* C$

c)

So one is first order rate constant using the lab data that is case a that is something that we looked at. For example, we considered the batch reactor and so on and so forth we calculated that. So we are going to look at that. Second case is using field data with the assumption of plug flow, okay. And the third one to be with the assumption of advection and dispersion. For advection-dispersion, obviously which model can you fit?

(Refer Slide Time: 09:57)



Advection-Dispersion System with First-Order Loss at Steady-state

$$C = C_0 \frac{4a\exp\left(\frac{Pe^+}{2}\right)}{(1-a)^2\exp\left(\frac{aPe^+}{2}\right)-(1-a)^2\exp\left(-\frac{aPe^+}{2}\right)}$$

$$a = \sqrt{1+\frac{4k\tau}{Pe^+}} = \sqrt{1+\frac{4kD}{(u^+)^2}}$$

$$Pe^+ = \frac{u^+x^+}{D}$$

$$\tau = \frac{x}{u^+}$$

$$u^+ = \frac{Q}{\varepsilon A}$$

$C = C_0 f(x)$

Dispersion co-eff.

: seepage vel.

You will have to fit this particular model, right. So for case a, which is case a here, case b here and case c here. Case a, what are we going to look at? We know that we came up with dc/dt=-k*C or Ct=C0*e power -k*t, right. So this is the one for the microcosm studies. And for b, it was a plug flow reactor. See that plug flow reactor, obviously advection is going to be there and you are going to have adsorption-desorption.

And in that case, we have looked at, I believe, dc/d tau=-k*C, right, that is what we looked at. And for c, the model is? This is the model out here, right. Again how is C changing with x. But here, D is the dispersion coefficient, right. This is something that we looked at, let us say. And typically this Pe, Peclet number, gives us an idea about the ratio of, let us say, the contaminant being transported by advection to that by dispersion.

Typically, to understand, let us say, which particular mode of transport is relatively the predominant, you look at the Peclet number. Numerator typically gives you an idea about the transport due to advection. The denominator gives you an idea about the transport due to dispersion and diffusion, let us say, right. Again coming back to here. So we are going to have to look at a, b and c cases.

So hopefully for today, we will have the time to be able to done with this. We done with at least case a. What are some of the aspects that we have? So here we have organic carbon partitioning coefficient for TCE. So this is something like KOC. And why is this relevant? We know that q=Kp*C. What is q? concentration of the relevant particular contaminant on the soil. C is the concentration of the particular contaminating the ground water, right.

We know that both of them are in equilibrium. And how are we relating them? We are using this particular variable Kp or the partitioning coefficient. But to what particular aspects or compounds on the particular soil is it that the contaminant is being adsorbed on to, right. What drives this adsorption now, right? Here as you know TCE is hydrophobic, right.

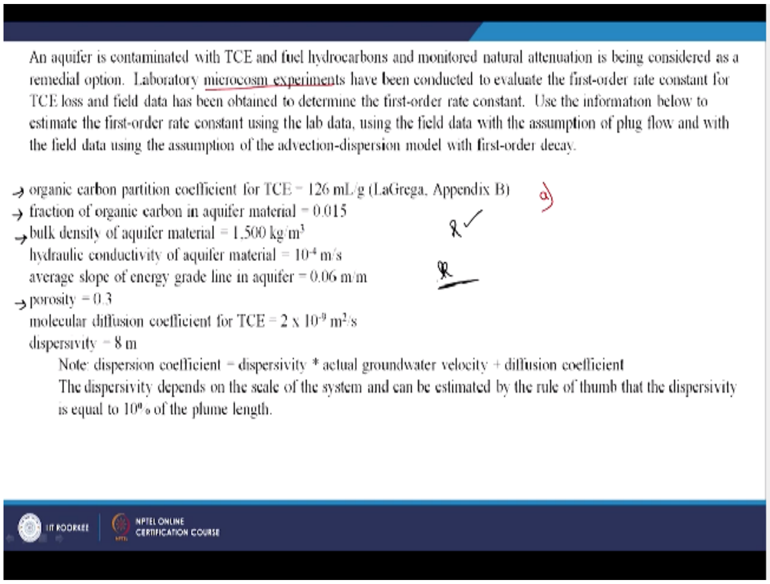
And any organic matter in the soil, right, if there is any organic matter present in the soil, obviously this particular TCE would not want to stay in water but would want to stay in that particular organic phase or be adsorbed on to that organic fraction. So that is why, let us say, this particular Kp can also be obviously further written as K*OC*fraction of organic carbon. So this is the partitioning between organic carbon, right and this is the fraction of organic carbon*concentration.

What does this tell you more or less? It is that the amount of organic content present in the soil is the relevant aspect that drives your particular partitioning as in. If you see that there is a 4C, the fraction of organic content present in your soil. If your 4C is higher, what does that mean? q is also higher, right. Again looks like fraction of organic carbon in aquifer material is just 0.015, bulk density of aquifer material is also given rho b, right.

Hydraulic conductivity is also given of aquifer material, right. Average slope is given. Porosity is given. Obviously using these, you can calculate the velocity or the Darcy's velocity, right, u=, I believe, Ki, right. Porosity is given. Molecular diffusion coefficient is also given, right. And dispersivity is given. So, I guess, this is going to be relevant to your particular kC, right. And here we are saying that dispersion coefficient can be calculated by empirical formula, dispersivity*actual ground water velocity + diffusion coefficient.

As we mentioned earlier, dispersion is due to 2 effects. As in one is due to the tortuous path of the ground water and also obviously you are going to have to take into account diffusion too. So that is what you see here. This dispersion coefficient takes into account both the diffusion coefficient and this particular tortuosity here, right. And then, more or less, you can look at this particular case and so on and so forth. And let me erase this here.

(Refer Slide Time: 14:29)

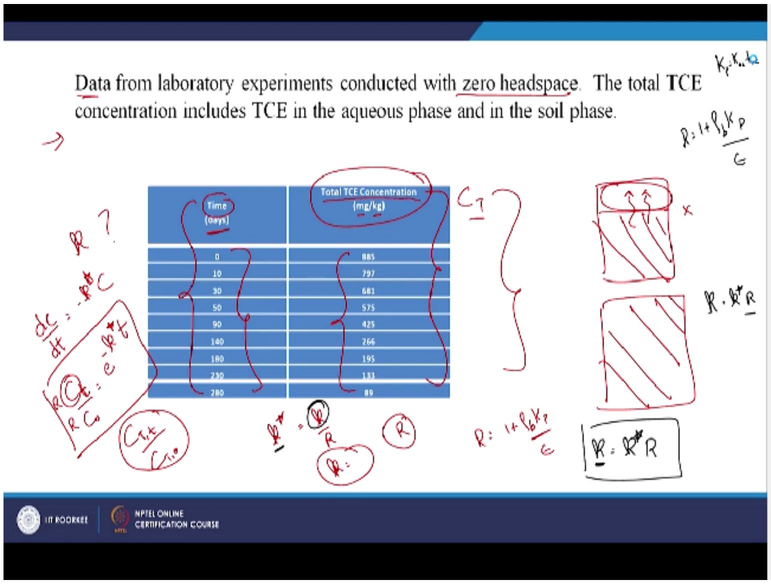


An aquifer is contaminated with TCE and fuel hydrocarbons and monitored natural attenuation is being considered as a remedial option. Laboratory microcosm experiments have been conducted to evaluate the first-order rate constant for TCE loss and field data has been obtained to determine the first-order rate constant. Use the information below to estimate the first-order rate constant using the lab data, using the field data with the assumption of plug flow and with the field data using the assumption of the advection-dispersion model with first-order decay.

organic carbon partition coefficient for TCE = 126 mL/g (LaGrega, Appendix B)
fraction of organic carbon in aquifer material = 0.015
bulk density of aquifer material = 1,500 kg/m^3
hydraulic conductivity of aquifer material = 10^{-4} m/s
average slope of energy grade line in aquifer = 0.06 m/m
porosity = 0.3
molecular diffusion coefficient for TCE = 2 x 10^{-9} m^2/s
dispersivity = 8 m
Note: dispersion coefficient = dispersivity * actual groundwater velocity + diffusion coefficient
The dispersivity depends on the scale of the system and can be estimated by the rule of thumb that the dispersivity is equal to 10% of the plume length.

You are okay? So now we are obviously going to look at case a now. What is case a? We just have the microcosm experiments. So first let us look at that data.

(Refer Slide Time: 14:38)



Data from laboratory experiments conducted with zero headspace. The total TCE concentration includes TCE in the aqueous phase and in the soil phase.

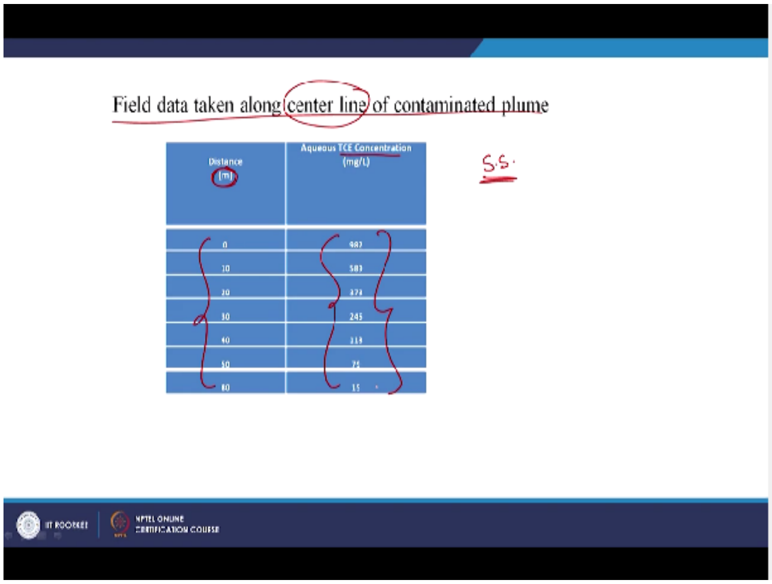
Time (days)	Total TCE Concentration (mg/kg)
0	885
10	797
30	681
50	575
90	425
140	266
180	195
230	133
280	89

So data from the lab experiments conducted with 0 headspace as in. So if this is my container and this is my aquifer media which I got from the relevant, what is it now, aquifer or the particular site, right. I cannot have headspace here. Headspace is that free space, let us say, if I can call that here. Why is that? Because, let us say, TCE, let us say, or even hydrocarbons, they are volatile, right. So if you have this particular headspace in your particular laboratory setup, what will happen?

The particular contaminant will not just change phase from water to soil but will change phase probably from water to the gas, right. The contaminant can volatilize. So you do not want to have this. So you want to have a case where you have no headspace, right. It is either just soil or ground water or water in this particular microcosm stage, right. That is one aspect. So what did they do?

They looked at the change of the relevant total TCE. They looked at C total, keep that in mind, with time, right. So they have time in days and mg of that particular contaminant per total mass, let us say, C total and they have the relevant data here, right. So how do we go about analyzing this. Before we go for this, let us also look at path b of the other data.

(Refer Slide Time: 15:55)



Field data taken along center line of contaminated plume

Distance (m)	Aqueous TCE Concentration (mg/L)
0	982
10	583
20	373
30	245
40	113
50	75
80	15

S.S.

So in this case, we have field data taken along the center line of the contaminated plume, along the center line. So we are assuming that it is representative more or less. So obviously here we are assuming that it is at steady state, okay. So the concentration does not change with time but what does it change with? It obviously changes with distance in plug flow or in ground water as the contaminant is being transported by the particular soil, right, not soil, pardon me, ground water.

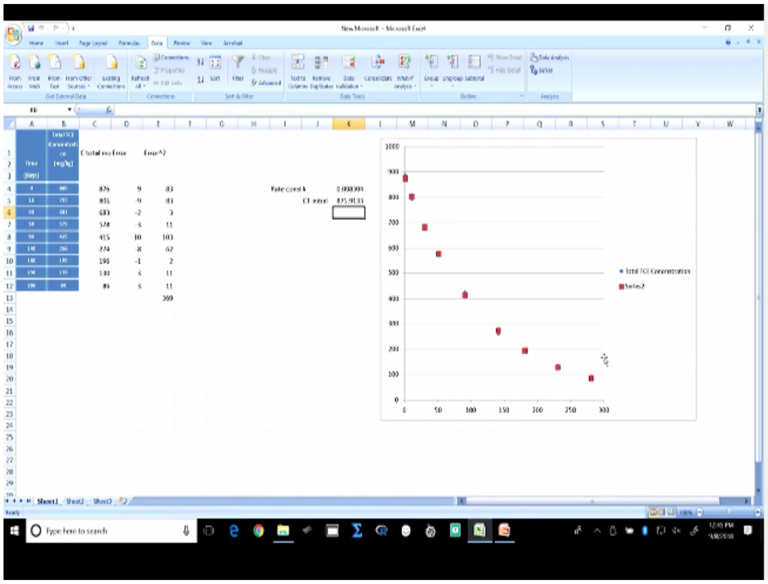
What is it, how is the TCE going to change? The TCE is going to change with distance, right. And that is what you see as the distance increases, you see that the concentration of that particular contaminant in the ground water is decreasing, right. And same case here too. Here you see that with increase in time, the concentration of TCE, total TCE is decreasing. Why is that happening?

So that means that there is some microbial activity that is leading to loss of this particular TCE in this laboratory or microcosm study. And in the second case, let us say, what could be causing this particular loss? It could be either, let us say, just advection or certainly, not certainly or your, and/or microbial activity, right. So for today, I believe, we are going to look at this particular case, data from the laboratory experiments and we are going to try to calculate, what did they ask for, the rate constant k.

How do I go about that, right? I know that dc/dt=-k--C, right or C at time t/C0=e power -k--*t, right. So if I fit this model to this particular data, I can get k-- and I know k--=k/R and I can calculate retardation factor from what I have and R is nothing but 1+rho bKp/porosity, right. So from this, I can calculate the first order rate constant, right. But one minor aspect that obviously we need to look at is here they gave the total concentration.

And here as you can see, here the C is the concentration of TCE in the aqueous phase. That is how we, if you remember the relevant variables, that is how we solve for it. But it is a minor aspect because as you see if I multiply the numerator and denominator by R, what will I have? The C total at time t/C total initially, right. So even if I have C total, I can still get this done, right. So obviously we need to move on to excel and be able to calculate that. So let us now switch to excel.

(Refer Slide Time: 18:34)



So here I have the relevant data in excel, right. So I have time and days and I have concentration, total concentration of TCE in mg/kg and we have that here, right. So obviously I need to fit this model to Ct/C0=e power -kt or multiplying the left hand side by retardation factor C total at time t/C total at time 0=e power -kt, right. So let us say I am going to look at 2 different aspects, right. So what are they? I will assume some rate constant.

So let us say this rate constant, let us say, is k here, let us say, or k is something like 0.005, let us say. This is just while learn initially obviously and using that, I can calculate a particular C observed, not C observed, C modelled, right. C total modelled, let us say, right. C total modelled and that is equal to, also I am going to assume some initial value of C total, C total initial, right. So that is for example for the trial, initial trial, I am going to go with the same concentration as is observed in the relevant data, right.

So this column is the observed data and I am trying to calculate the modelled data. How am I going to do that? I am going to assume some value of C total initial and some value of rate constant, right. So that is equal to Ct=C0, C0 will be this. So the dollar symbol to keep that cell constant, right, *exponential or e to the power of -k*time, right. So that is what I have here and this k4 needs to be held constant, right. k is the same. So for this k value, let us say, and for this C total initial value, I have to be able to model this.

As you see, this particular k value does not really explain the data well, right. As you can see 885, yes, obviously initial value. But as you can see the final value is far off from this particular value at time=280, right. And obviously all the other values too are nowhere near the actual observed values, right. So now what do am I going to do? My objective is to change k and C total initial such that the error between these 2 particular observed and modelled values will be minimum, right.

So what is the error here? I will label that as error. So that is equal to C modelled-, or C observed-C modelled, right. And I am going to drop that here. So I have this, right. Obviously as you can see, everything is negative. What does that mean? That my model is overestimating the relevant data, right. Overestimating the relevant variable, pardon me. This is the error. And obviously I am going to look at error to the power of 2, error square, right.

So error square, so that is equal to the cell to the power of 2, yes. And I am going to do that and now I am going to calculate the sum of squared errors that is equal to the sum of all these squared errors, right. So I end up with this. As you can see what am I trying to do or what is the objective here? I want to get that value of rate constant and that value of C total initial that will minimize the sum of squared errors, right.

So that will be my true value of or relatively better value of k and C total initial. How do I do that? Obviously I have different ways to get that done. One is here, go to data, go to solver. So here as you see, you can have different aspects here. So what does this, what do we have here? We have, let us say, the target cell and the target cell in this case is this cell, sum of squared errors.

And what are we trying to do? We are trying to minimize that sum of squared errors. So the target cell, we are trying to minimize that. And how are we trying to minimize that? By changing these 2 cells. So what am I asking excel here to do? I am asking excel to change the values of rate constant and C total initial, right in such a way that this particular cell of sum of squared errors is going to be the minimum, right.

So I am going to ask you to solve, okay. And now excel solved for it and now gave me a new value of rate constant and that is equal to 0.008. And I think because it is the first order loss, it is going to be day inverse, right, day inverse as you can see here. And C total initial, the true values used to be 876 or so though. So there are 2 ways to go about it. Either you can keep C total initial to be actually 80 85 and just change k or you can model this too.

So let us just try to plot this in the first case. So plot, okay, so this did not take the data well, right. So x values should be the time, y values should be these concentrations. And as you can see, this is the actual, what do we say, data, the observed data, right. Let us also try to plot the model data. So select data, add and x values are still going to be time and y values are going to be the modelled data, right.

So I am going to model that. As you can see here when I overlay this, I see that the model and the observed values almost overlap each other. So that means obviously you can understand that, it is a pretty good fit, right. That is one aspect to look at. So for example though if I change k, let us see how this system changes, right. So the red dots are the observed data points and the blue dots are the actual data points, right.

And let us try to get that. So let us change 0.008, let me just go with 0.005 as I calculated earlier. So now as you see my model, this is my model. The red data points are not doing a good job. They are pretty far off or the error is considerable. This is the error. The difference between these 2 values is considerably high when compared to the observed values, right. So let me go to a higher value, 0.00 or 0.01.

So now you see the model has moved in the other particular direction. Now it is overestimating everything I guess or underestimating it or seeing that it is pretty fast, right. You see that. So what am I trying, doing here? I am just changing the rate constant here. Earlier it was 0.008 which was the true value from the solver. When I changed it to different values, you see that the model moves away from the observed values.

But what am I trying to do? I am trying to get it done in such a way that this modelled value will be pretty close or the sum of squared errors will be minimum to the particular when compared to the observed values. So let us do that again. So I am going to go back to this particular data, solver. How do I do that? I am asking it to change the sum of squared errors to the minimum by changing cells like rate constant and C total initial and ask it to solve.

And again obviously I get this particular answer, 0.008 304 day inverse, right, which gives me an idea that, not which gives me an idea, it obviously is the best fit for this particular data. So again this is obviously called regression too, right. So here we just calculated the rate constant, let us say. And but is it true rate constant? Not really. This was the one for Ct/C0=e to the power of or Ct=C0*e to the power of -k*t, right.

So here we calculated k*. k*=k/the retardation factor. So actual retardation, actual rate constant is this particular rate constant*retardation factor, right. Let us just check that once here. So we have, what did we calculated here? So we just calculated k-- here, right. So how do I get k? Obviously I can get k by k=k-- which I calculated, *the retardation factor, right. So when I do that, I can calculate my k.

This is the way I write k, please pardon my handwriting skills, right. k=k--*the retardation factor and you can calculate R. R=1+rho bKp/porosity. Kp is nothing but as we mentioned KOC*FOC. Let us see if we have all the data. So Kp or bulk density, yes, bulk density is given. Porosity is given. KOC is given and FOC is given. So thus I can calculate the R. Once I calculate R, I can calculate the actual rate constant, right. I guess, I am out of time for today.

But again well let us just summarize the approach. What did we do? We had the data of the, what do we say, from the experiment where we measured the change in concentration with time. That is what we had. And then we assumed some value of k and C total initial and calculated the relevant observed, not observed, pardon me, the modelled values, right. That is what we did here. Let me try to switch here.

So we assumed some value of k, some value of C total initial and then calculated the modelled value, right, initially. Again there are 2 ways obviously as I mentioned. You can either assume that C total initial is constant. Typically let us say, that is a descent way to go about that. But here I assume that there might be errors in even the C total initial that you measured so that is why I kept that to be a relative variable here.

Or that is something that needs to be found out from the relevant data too, right. But typically you will have greater, what we say, confidence in the initial data point that you are measuring. So typically you can keep that constant, that is up to you, right. But here I can kept 2 variables here. And I calculated the error first and then the sum of squared errors. And then used data solver to minimize this sum of squared errors.

What is it now? So that my particular model can approximate my particular data or observed data in the best possible manner or by minimizing the sum of squared errors. Again that is more or less regression now. So in which particular case would you have greater confidence. Let us say case a you have only 2 or 3 data points. Case b when we have around, let us say, 9 data points, let us say, right.

In which case will you have more confidence in your particular ability to calculate or estimate that rate constant. Obviously the greater the data, right, the greater the number of data points, the greater the confidence, let us say, if I can say so. Less number of data points, let us say, the greater the chance of errors in estimating k. So typically the greater the number of data points, the better but obviously you will have some particular upper threshold obviously, right.

Otherwise, you cannot obviously get done with your experiment in a feasible manner, right. So again with that we will end today's session. And in next session, I guess, we are going to look at the case b where we have plug flow and so on and so forth. And thank you. That is, it for me for today.