

Spring 2005

Homework #5

Due Wed., March 2, 2005

University of South Florida

Civil & Environmental Eng.

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- (1) Suppose that some DDT is released into an aquifer. (DDT is a pesticide that has been banned in the U.S. but is still used in some parts of the world, particularly where mosquito-borne disease is a health hazard.) The octanol-water partition coefficient for DDT is $K_{OW} = 10^{4.96}$, and the aqueous solubility of DDT is $5 \mu\text{g/L}$. The aquifer is comprised of silty sand, with hydraulic conductivity $K = 10^{-4}$ m/s, porosity $n = 0.3$, hydraulic gradient 10^{-3} , longitudinal dispersivity $\alpha_L = 10$ m, solid density $\rho_g = 2500$ kg/m³, and organic carbon content $f_{OC} = 0.001$.
- Suppose that the sorption process is rapid and the isotherm is linear. Calculate the retardation coefficient, R , for DDT transport in the aquifer. (Hint: use an appropriate relationship based on K_{OW} .) Explain how R influences DDT transport, dispersion, and reaction. Discuss briefly the environmental relevance of the value of R that you calculated for DDT.
 - Estimate the travel time for DDT to be transported a distance of 100 m under the conditions given above.
 - Estimate the plume length, L_x , of the DDT plume at the time calculated in part (b), above. Assume that the DDT mass was initially introduced as a short, rapid pulse. A good way of defining L_x is the region that is within ± 2 standard deviations (i.e., $\pm 2\sigma_x$) from the center of the plume.
 - Estimate the Peclet number, Pe , for the conditions above.
 - Let's see if degradation can be ignored, or if it is significant. Assume Monod kinetics for the degradation of DDT. Suppose that the concentration of bacterial cells in the aquifer is $X = 0.1$ mg cells/L, the maximum specific utilization rate is $k' = 0.5 \times 10^{-6}$ mg DDT per mg cells per day, the half-velocity concentration is $K_S = 0.5$ mg/L, and the DDT concentration is around the aqueous solubility, $5 \mu\text{g/L}$. Estimate the fraction of DDT mass that remains once the plume has traveled 100 m. Is it OK to ignore degradation over this travel distance?

Hint: for parts (b)–(e), be sure that the answers you calculate are consistent with what you wrote in your discussion for part (a).

- (2) This is a question that I gave on a final exam for a class that I taught at Stanford University during summer 2003. The class was *not* Transport in Porous Media, but we did cover contaminant transport in groundwater to some extent. This would probably make a good exam question for CGN 6933, but I have decided to give it as a homework problem instead. Here it is:

The one-dimensional (longitudinal) transport of a contaminant in groundwater is often described with the following equation:

$$\frac{\partial C(x, t)}{\partial t} = \frac{D_x}{R} \frac{\partial^2 C(x, t)}{\partial x^2} - \frac{v}{R} \frac{\partial C(x, t)}{\partial x} - \frac{k}{R} C(x, t)$$

(2) continued

- (a) Identify the physical processes accounted for by each of the three terms on the right-hand side of the equation. Describe the physical meaning of the retardation coefficient, R , and why it appears in this equation.
- (b) The above equation was derived by invoking the Local Equilibrium Assumption (LEA). Explain briefly what this assumption is, and under what conditions you would expect it to be valid.

In the 1980's, researchers from Stanford University and from the University of Waterloo conducted an experiment that is now very famous in the area of contaminant transport in groundwater. These researchers injected seven compounds into the groundwater at an aquifer in Canada, then monitored the fate and transport of the seven compounds over the following 3 years. The aquifer is called the Borden aquifer, so the experiment is now known as the Borden experiment.

The seven compounds were: Chloride (Cl-), Bromide (Br-), Carbon tetrachloride (CT), Bromoform (BF), Perchloroethene (PCE), Dichlorobenzene (DCB), and Hexachloroethane (HCE).

Table 1: Selected Properties of Chemicals Injected during Borden Experiment

	MW (g/mol)	K_{OW}	C^{SL} (g/L)	P^{sat} (torr)	D^{molec} (m ² /sec)
Cl-	35.45				2.0×10^{-9}
Br-	79.90				2.0×10^{-9}
CT	153.8	540	0.97	115	
BF	252.7	200			
PCE	165.8	760	0.15	19	0.79×10^{-9}
DCB	147.0	2400	0.115	1.5	
HCE	236.7	4000			

- (c) Researchers found that Cl- and Br- behaved conservatively; CT, BF, and PCE were persistent but not conservative; DCB and HCE were not persistent. Briefly explain (in your own words) what is meant by “conservative” and “persistent” in this context. What does this tell you about the behavior of Br-? about the behavior of CT? about the behavior of DCB?

(2) continued

- (d) The seven chemicals were added as a finite pulse over a time span of 14.75 hours. Suppose we approximate this as an instantaneous pulse. Then, what would be the solution to the partial differential equation from part (a) of this question? In other words, what would be the concentration $C(x, t)$ of any particular compound? (Hint: for boundary conditions, you may assume that the aquifer is long in both the upgradient and downgradient directions.) Do you think it is valid to approximate the chemical addition as an instantaneous pulse? Why or why not?

Table 2: (Average) Properties of the Borden Aquifer

Hydraulic conductivity, K_H :	8.2×10^{-5} m/s
Hydraulic gradient:	0.0043
Longitudinal dispersivity, α_L :	0.1 m [remember $\alpha_L = D_L/v$]
Porosity, n :	0.33
Grain density, ρ_g :	2.5 g solid / cm ³ solid
Fraction of organic carbon in sediments, f_{OC} :	0.001

- (e) Estimate/calculate the retardation factor, R , for Br-, CT, and DCB.
- (f) Estimate/calculate the distance traveled by the Br-, CT, and DCB plumes in the first 1 year after injection.
- (g) Estimate/calculate the length of the plumes (i.e., the plume spread in the longitudinal direction) for Br-, CT, and DCB after 1 year of travel.
- (h) On the attached figure (next page), draw a map of the Br-, CT, and DCB plumes at a time $t = 1$ year after injection. Assume that the plume spread in the transverse direction (i.e., the direction perpendicular to the flow direction) is 10% of the spread in the longitudinal direction. Indicate clearly which plume is for which compound. Briefly explain (1–2 sentences) how the chemical transport depends upon the chemical properties.
- (i) Be sure to turn in the figure with your assignment.
- (3) About how long (measured in hours) did it take you to complete this homework?

