

Spring 2005

Homework #8

Due Mon., April 11, 2005

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Civil &amp; Environmental Eng.

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Suppose you are investigating the transport of a hazardous chemical at a contaminated groundwater site. We'll call the contaminant "compound  $H$ " (for "hazardous"). You want to know how compound  $H$  behaves in the contaminated aquifer. In order to predict this, you conduct some experiments. The first experiment you conduct is to measure the sorption isotherm of compound  $H$  on some samples of aquifer sediment that you collected from the site. Table 1 shows the data you collected during your isotherm experiments.

Table 1: Sorption Isotherm Data for Compound  $H$ 

| aqueous<br>concentration<br>( $\mu\text{g}/\text{L}$ ) | sorbed<br>concentration<br>( $\mu\text{g}/\text{kg}$ ) |
|--|--|
| 7.1  | 160  |
| 18   | 320  |
| 32   | 480  |
| 77   | 840  |
| 180  | 1320   |
| 430  | 1950   |

The next experiment you run is to measure the transport of a *conservative tracer* through a column of the aquifer sediment. You take a column of length  $L = 50$  cm and fill it with uncontaminated sediments from the site you are investigating. After filling the column and saturating it with water, you estimate that the porosity is  $n = 0.3$  and that the bulk density is  $\rho_b = 1.8$  g/cm<sup>3</sup>. You set up the column in the lab, and you pump water through it with a specific discharge  $q = 1.5$  cm/d. At time  $t = 0$ , you start introducing bromide tracer at the front end of the column, at a constant concentration  $C_0 = 100$  mg/L. You purge the back end of the column, so that the bromide concentration at that end is always  $C(x = L) = 0$ . As the experiment progresses, you collect samples from  $x = 25$  cm (i.e., halfway through the column), and you analyze them for the concentration of bromide. Table 2 shows the data that you collected from this experiment.

Table 2: Bromide Concentration History at  $x = 25$  cm

| time<br>(day) | bromide<br>concentration<br>(mg/L) |
|---------------|------------------------------------|
| 0             | 0                                  |
| 0.5           | 0                                  |
| 1.0           | 0                                  |
| 1.5           | 0                                  |
| 2.0           | 0                                  |
| 2.5           | 0.9                                |
| 3.0           | 3.8                                |
| 3.5           | 13.4                               |
| 4.0           | 22.2                               |
| 4.5           | 43.7                               |
| 5.0           | 49.3                               |
| 5.5           | 70.7                               |
| 6.0           | 75.1                               |
| 6.5           | 87.6                               |
| 7.0           | 88.9                               |
| 7.5           | 96.6                               |
| 8.0           | 94.4                               |
| 8.5           | 98.8                               |
| 9.0           | 98.0                               |

- (1) Now suppose that, instead of bromide tracer, you had compound  $H$  being added to the front end of the column. Assume an inlet concentration  $C_0 = 1$  mg/L – note this is different from the inlet bromide concentration. Here is your assignment: Write a computer program to predict the concentration history of compound  $H$  at the location  $x = L/2 = 25$  cm. You may assume that the Local Equilibrium Assumption is valid for compound  $H$  as it travels through the column. Hint: Use the experimental data to determine the necessary physical and chemical parameters for your prediction. Another hint: based on Table 1, the sorption isotherm does not appear to be linear.

Submit your code and a graph of the concentration history. Also submit a short write-up of any important parameter estimates you made, or assumptions you made, or calculations you performed, etc. With your write-up, you should include any pertinent graphs or figures. I am not looking for a 50-page write-up, but I do want to be able to understand your approach to solving this problem. Your write-up should be sufficient that somebody could use it to verify all your estimates and calculations.

- (2) One might wonder why somebody would perform sorption isotherm experiments and tracer transport experiments in order to predict the transport of compound  $H$ . Why not just run a column transport experiment with compound  $H$ , and take the experimental data? Then you get the right answer, and you needn't bother doing all these calculations

based on “indirect” experiments. However, I can think of at least one good reason why the approach outlined above is a logical one, and might be preferable to running a transport experiment with compound  $H$ . Can you think of a good reason to proceed in the manner described, rather than just running compound  $H$  through the column directly? Hint: compare the experimental data in Table 2 to the concentration history you predicted for compound  $H$ .

(3) About how long (measured in hours) did it take you to complete this homework?

By the way, the data analysis and the predictions that you perform in this problem are very realistic. Interpreting sorption isotherm data, and fitting a model to experimental data, and predicting transport of a sorbing contaminant – these are all things that engineers and hydrogeologists perform on a pretty regular basis.