CEE 348: Contaminant Transport in Groundwater

(Lab adapted from a program at the University of Texas.)

OBJECTIVE:

This laboratory is designed to acquaint you with some of the hydrogeological principals important in evaluating the transport of solutes and contaminants by groundwater. These principles apply whether or not the solutes are naturally occurring or are contaminants.

BACKGROUND:

The relationship between advection and dispersion is used to determine the transport of mass in porous media. Generally, the bulk transport of fluids, and solutes, is dominated by advection and dispersion. Diffusion is usually lumped in with the advective and dispersive behavior of fluids. Longitudinal dispersion is what causes contaminant plumes to spread out in the direction of flow. The spreading is due to heterogeneity in the medium, such as a distribution of pore sizes (and shapes). Dispersion perpendicular to the aquifer flow direction is called transverse dispersion. It is related to diffusion and plays an important role in the remediation of contaminants. It helps to dilute their concentration and to mix the contaminants with reactive compounds and microbes in the soil.

The dominant process of mass transport is advection moving aqueous chemical species along with fluid flow. Therefore, most contaminant modeling begins with advective transport. While these modeling attempts can be valuable in terms of determining travel times and capture zones, the influences of dispersion and diffusion remain understated. Distinguishing between the various flow mechanisms is still poorly understood—this limits our ability to model contaminant behavior. For now, calculations couple advection and dispersion as a single flow mechanism.

The majority of the following section is taken from "Solution to the advection-dispersion equation: Continuous load of finite duration" by Robert L. Runkel, 1996: Given specific initial and boundary conditions, the advection-dispersion equation describes spatial and temporal variations in solute concentration. A simple form of the governing equation known as the constant-parameter advection-dispersion equation may be derived for the case of steady, uniform flow and spatially constant model parameters. Analytical solutions for this simplified form are widely available (for example, see Ogata and Banks, 1961).

Published analytical solutions for the constant-parameter advection-dispersion equation generally consider two input loading scenarios. Under the first scenario, a finite amount of mass is instantaneously released at the upstream boundary of the modeled system. This type of input function is applicable when the solutes of interest are introduced into the system over a short period of time, such as with a slug injection of dye. In the second input scenario, solutes are continuously released into the system at the upstream boundary.

We consider a system in which physical transport is primarily one-dimensional—that is, solute concentrations are horizontally and vertically well-mixed so that concentrations vary only in the longitudinal or downstream direction. In addition, a steady, uniform flow field is imposed; the effects of dispersion are spatially constant; and the solutes are conservative. Given these assumptions, conservation of mass yields the constant-parameter advection-dispersion equation:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} \quad (1)$$

where: C = concentration [ML-3];
t = time [T];
v = the average seepage velocity [LT-1]; (Recall, the average seepage velocity is the same as the average linear velocity of a contaminant and equals the Darcy velocity divided by the effective porosity.)
x = distance along the flowpath [L];
D = coefficient of hydrodynamic dispersion [L2 T-1].

For the case of a continuous source of infinite duration, the initial and boundary conditions are
given by:

$C(x,0) = 0$ for $x \geq 0$
$C(0,t) = C_0$ for $t \geq 0$
$C(\infty,t) = 0$ for $t \geq 0$ (2)

where C_0 = concentration at the upstream boundary [ML-3].
The analytical solution is given by (Ogata and Banks, 1961):

$$C(x,t) = \frac{C_0}{2}\left[erfc\left(\frac{x-vt}{\sqrt{4Dt}}\right) + exp\left(\frac{vx}{D}\right)erfc\left(\frac{x+vt}{\sqrt{4Dt}}\right)\right] \quad (3)$$

where erfc is the complementary error function, a mathematical function derived from basic statistics, defined as:

$$erfc(x) = \frac{2}{\sqrt{\pi}}\int_x^{\infty} e^{-t^2}dt = 1 - erf(x) \quad (4)$$

MS Excel has both the error function and the complementary error function.
Simplified forms of (3) are often presented in the literature. Ogata and Banks (1961) state that the omission of the second term in (3) results in a maximum error of three percent for values of $D/vx < 0.002$. We will use the simplified form of

$$C(x,t) = \frac{C_0}{2}\left[erfc\left(\frac{x-vt}{\sqrt{4Dt}}\right)\right] \quad (5)$$

REFERENCE:

Ogata, A., and Banks, R.B., 1961, A solution of the differential equation of longitudinal dispersion in porous media: U.S. Geological Survey Professional Paper 411-A.

QUESTIONS:

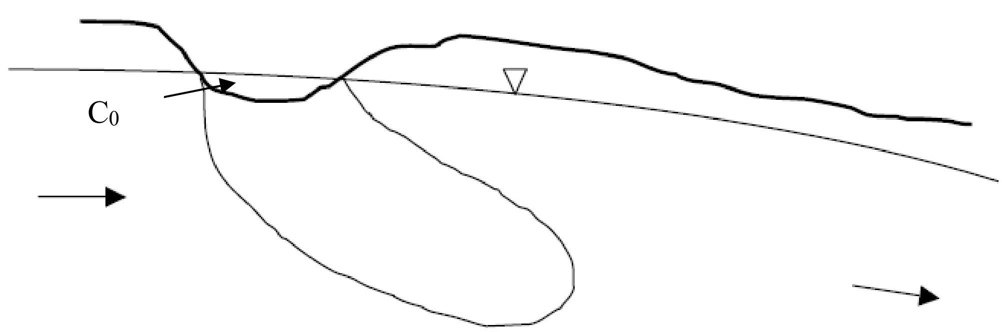
1. What are the three processes which affect the flow of solute in groundwater?

2. Define molecular diffusion.

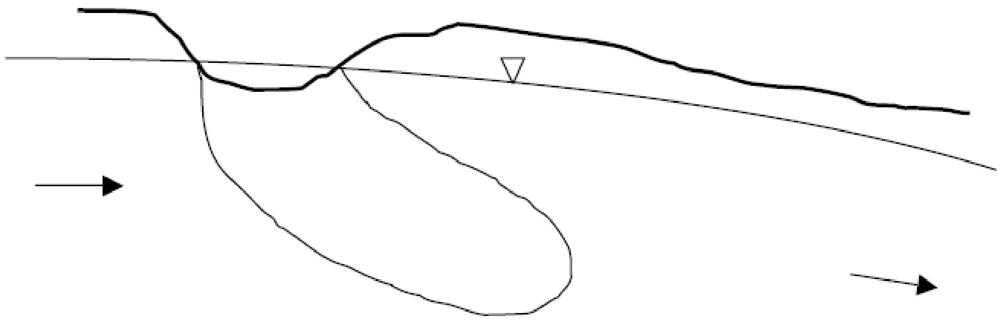
3. Define mechanical dispersion.

4. A series of diagrams showing a contaminant plume are given below. The source represents the initial concentration, C_0. For each scenario below sketch concentration contours on the diagram given representing relative concentrations (C/C_0) of 100% and 50%. Also, draw a breakthrough curve for that scenario on the axes given. Put an **X** on the diagram, somewhere in the lower-right side, for the location where you are showing the breakthrough curve. Arrows show direction of groundwater flow. Note also that the contaminant is heavier than water and so is also sinking due to gravity. The intersection of the groundwater level with the heavy solid line is C_0 for all cases (shown in (a)).

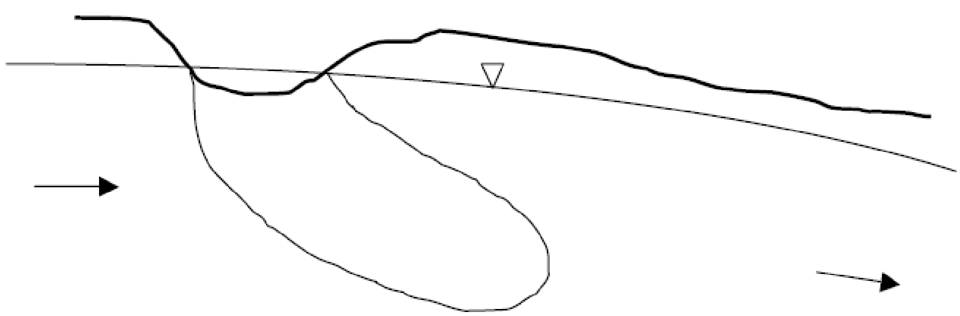
a) Plug flow (no dispersion). No need to draw concentration contours for (a), only the breakthrough curve. HINT: The solid line and everything inside it is C_0 for this case.



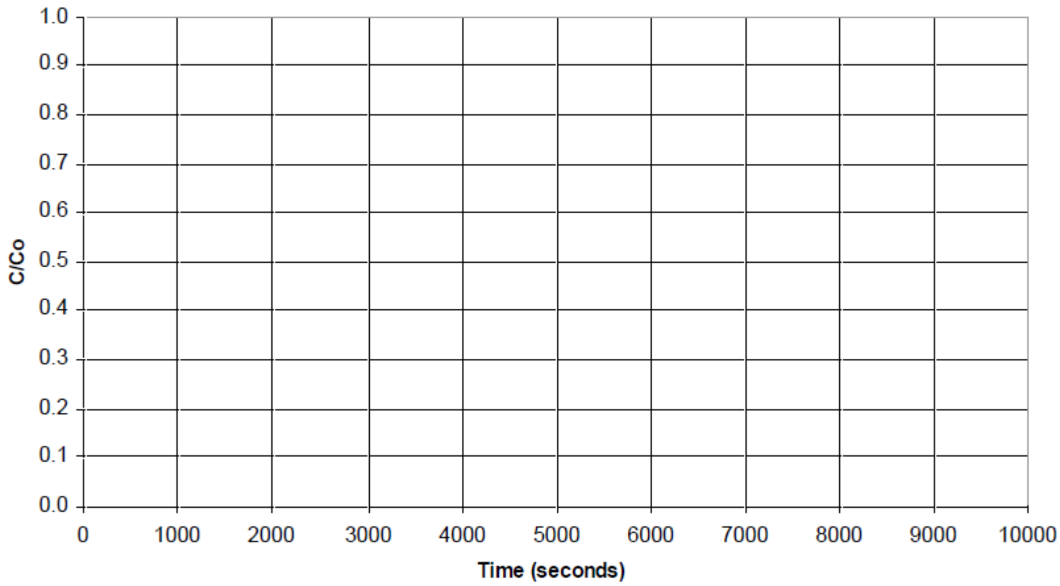
b) Advection and dispersion (happening in all directions). In this case the heavy solid line indicates C/C_0 of 0.5.



c) Same as (b), but add radioactive decay of the contaminant.



5. a) Consider a sand tube of diameter 12.0 cm and an effective porosity of 39.0% that is transmitting flow at a rate of 1.16 cm^3/s. Calculate the relative concentration (C/C_0) at a distance of 1.0 m down the length of the column using the Ogata and Banks solution. For this, please modify and use either the **Matlab code or the Excel sheet** provided. Plot relative concentration versus time over a range of times such that the entire breakthrough can be seen for two different coefficients of hydrodynamic dispersion: 1.0 x 10^{-5} m^2/s and 1.0 x 10^{-6} m^2/s.



b) Now that you have plotted the breakthrough curves for these two solutes, consider their physical behavior in the environment. What if an industrial manufacturer spilled these two solutes into an aquifer that also serves as a water supply? Your job is to monitor their concentration in a down-gradient monitoring well. Based on your breakthrough curves, discuss what you expect to see. For example, which solute will appear first? Which will remain the longest? If you find the opposite, what might be the explanation?