Physical and Chemical Hydrogeology

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Any attempt to interpret mass or contaminant distributions or to analyze a problem quantitatively requires estimates of the important transport parameters. In this chapter, we will examine the variety of field and laboratory techniques available for this purpose and discuss their problems and limitations. This knowledge provides the parameter-based framework that is essential for designing field studies. The variety of different chemical processes often means that any one of several reactions might affect dissolved contaminants in surprisingly similar ways (for example, mineral precipitation and cation exchange, or sorption and bacterial reduction). Thus, identifying processes or combination of processes can be a difficult and not insignificant problem. At sites of ground water contamination, predictions of contaminant behavior or choices for remedial strategies depend on understanding the geochemical processes.

There is often the need to go one step beyond identifying a process to characterizing it in terms of equilibrium constants or kinetic terms. For example as we saw in Chapter 17, such information is absolutely necessary for contaminant transport models. In many respects, this investigation of geochemical processes is a new area for most practitioners. Parameters are required to characterize processes like hydrophobic sorption and organic biodegradation, which a few years ago many people really never even knew existed.

18.1 *Tracers and Tracer Tests*

Because tracers reflect the outcome of mass transport process, they are useful for characterizing mass transport and mass transfer processes. The most important tracers are (1) ions that occur naturally in a ground water system such as Br^- or Cl^-; (2) environmental isotopes such as ^2H, ^3H, or ^{18}O; (3) contaminants of all kinds that enter a flow system; and (4) chemicals added to a flow system as part of an experiment. This last group could include radioisotopes such as ^3H, ^{131}I, ^{82}Br; ionic species such as Cl^-, Br^-, I^-; and organic compounds such as rhodamine WT, lissamine FF, and amino G acid. Many of these ions or compounds do not react to any appreciable extent with other ions in solution and the porous medium. These are what classically have been referred to as "ideal tracers." Others do react and for this reason are particularly useful in defining the nature of reactions. Excellent reviews of ground water tracers are given by Davis and others (1985) and Smart and Laidlaw (1977).

Given this choice of tracers confusion can arise as to which to use. In most cases, the choice is linked inexorably to the scale of the study or the presence of a contaminant plume. For example, tracing flow and dispersion in a unit of regional extent (10s to 100s of km) will involve either naturally occurring ions or environmental isotopes. Conducting a tracer experiment on such a large scale is simply not feasible because of the long times required for tracers to spread regionally. On a more localized or site-specific basis (several kilometers), the presence of a contaminant plume that has spread over a long time automatically makes it the tracer of choice. Again, time is insufficient (except perhaps in karst) to run an experiment at the scale of interest. Only for small systems (for example, some fraction of a kilometer) is there any real justification for running a field tracer experiment. It is only for these experiments when a selection has to be made among the various tracers. For reactive tests, the best tracer is one that participates fully in the reaction of interest.

Tracers are transported in two kinds of flow environments. In a natural gradient system, tracers move due to the natural flow of ground water. In a system stressed by injection and/or pumping, transport occurs in response to gradients typically much larger than those in natural systems. A small-scale tracer experiment can involve either of these flow conditions.

Success in all these tests depends on adequately characterizing concentration distributions in space and time. Typically, a large three-dimensional network of monitoring points is necessary to define the tracer distribution accurately. Point sampling is essential to avoid concentration averaging within the well bore in cases where concentrations vary over relatively small vertical distances. For example, estimated values of dispersivity tend to be larger when the number of individual sampling points is small or samples are collected over relatively large vertical intervals. This excess dispersion represents error due to inadequacies of the sampling network.

Field Tracer Experiments

Field tracer experiments can be run with a natural flow system or one modified by pumping or withdrawal. It should be possible in theory to estimate mass transport parameters from almost any test where a tracer is added in a controlled way. However, a few more or less standard tests are preferred because in most cases there are simple procedures for interpreting the results. Unfortunately, many of these tests are subject to error because run in their basic configuration there is often an insufficient number of monitoring points to provide a three-dimensional representation of the tracer distribution.

Natural Gradient Test

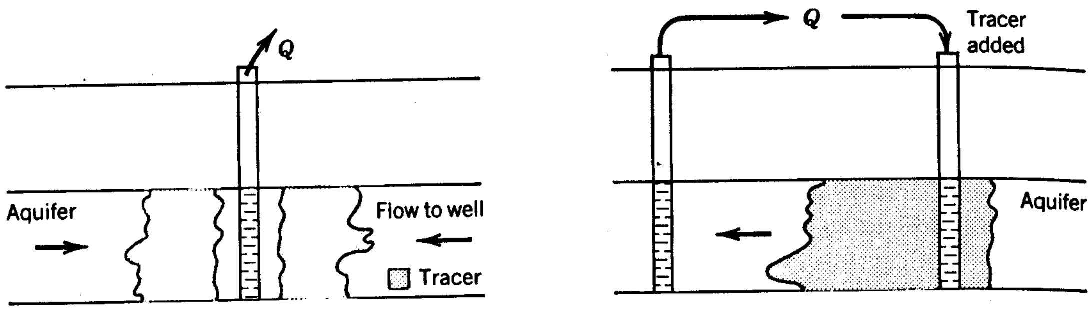
The natural gradient test involves monitoring a small volume of tracer as it moves down the flow system. Keeping the quantity of tracer small minimizes the initial disturbance of the natural potential field. The resulting concentration distributions are the data necessary to determine advective velocities, dispersivities, and occasionally equilibrium and kinetic parameters.

This experiment typically requires a dense network of sampling points. In one research study at Canadian Forces Base Borden, Canada (Mackay and others, 1986), the network contained more than 5000 separate sampling points. Not every experiment requires this kind of instrumentation. However, serious attempts at estimating transport parameters will require many tens to several hundred monitoring points.

Single-Well Pulse Test

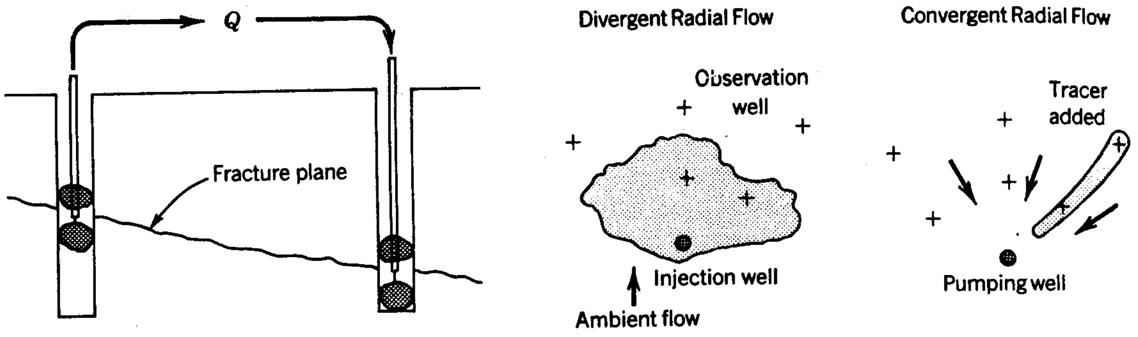
The single-well pulse test (Figure 18.1*a*) involves first injecting a tracer followed by water into an aquifer at some constant rate. After an appropriate period of injection, the aquifer is pumped at the same rate. The concentration of tracer in water being withdrawn is monitored as a function of time or total volume of water pumped. These concentration/time data provide a basis for estimating the longitudinal dispersivity and chemical parameters like K_d within a few meters of the well (Pickens and others, 1981). Fried (1975) describes a more refined version of this test where concentration/time data are collected at different positions in the well with a downhole probe.

While historically of some interest, this test has limited applicability in estimating values of dispersivity. It is generally not possible to scale up dispersivity



(a) Single-Well Pulse Test

(b) Two-Well Tracer Test



(c) Two-Well Tracer Test in Fractured Rock

(d) Single-Well with Multiple Observations Wells

Figure 18.1
Examples of field tracer tests.

measurements made at such a small scale to the larger scales of interest in most problems. In addition, the lack of detailed observations on how the tracer is spreading in the vicinity of the well makes any dispersivity estimate quite crude. This test holds more promise for evaluating geochemical processes. Because reactions operate on a local scale, there is no real scaling problem.

Two-Well Tracer Test

The two-well test involves pumping water from one well and injecting it into another at the same rate to create a steady-state flow regime (Figure 18.1*b*). The tracer is added continuously at a constant concentration at the injection well and monitored in the withdrawal well. The simplest way of running this test is by recirculating the pumped water back to the injection well as is shown on the figure. However, the tracer concentration will begin to increase at the injection well once breakthrough occurs at the pumped well. The test can also be run without recirculation by providing the water for the injection well from an alternative source. As before, the resulting concentration versus time data at the pumped well are interpreted in terms of processes and parameters. These tests can be conducted over several hundred meters in highly permeable systems. However with only a single monitoring point, the test provides at best only a crude estimate of dispersivity. Estimates can be improved by adding more observation wells between the pumping/injection doublet.

Modified versions of a two-well test have been conducted in fractured rocks (Raven and Novakowski, 1984). Packing off a small section of the borehole (Figure

18.1*c*) isolates a single fracture plane between pumping and injection wells. While this test is technically more demanding because it requires working with packers, it involves the same kind of interpretive technique and is subject to the same limitations we just discussed. In all cases, there is the inherent assumption of radial flow.

Single-Well Injection or Withdrawal with Multiple-Observation Wells These tests create a transient radial flow field by injection or withdrawal. The radially divergent test (Figure 18.1*d*) involves monitoring the tracer as it moves away from the well. The radially convergent test involves adding the tracer at one of the observation wells and monitoring as it moves toward the pumped well. Parameters can be estimated at scales of practical interest with reasonable accuracy provided a reasonable number of observation wells is provided. If a choice exists as to which of these two tests to run, the divergent flow test is preferable (Gelhar and others, 1985). The converging flow field (Figure 18.1*d*) counteracts spreading due to dispersion and is thought to be less useful.

18.2 The Diffusional Model of Dispersion

This section illustrates how the diffusional model of dispersion provides a basis for estimating dispersivities from concentration data. Concentration distributions are assumed to be normally distributed with the dispersion coefficient related to the variance of the tracer distribution and time and dispersivity related through velocity to the dispersion coefficient. A significant advantage of working with plume statistics alone is that dispersivity estimates are independent of the assumptions implicit in the advection-dispersion equation. As Freyberg's (1986) work at the Borden site showed, this method provides information on how dispersivities vary as a function of travel distance. In the following section, we will explore other approaches that involve fitting various forms of the advection-dispersion equation to concentration data. In most cases, interpretations based on these approaches require that dispersivities remain constant as a function of travel time (Freyberg, 1986).

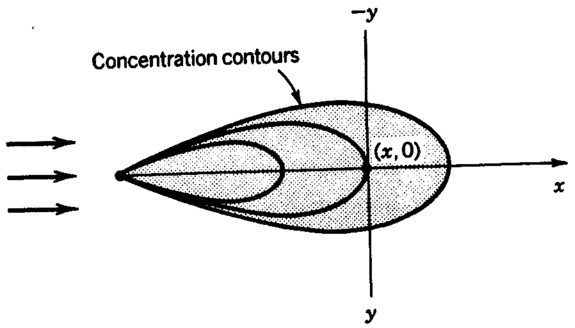
Consider the two-dimensional plume shown on Figure 18.2*a* produced by a continuous, point source. At any point along the middle of the plume (for example, x,0) a breakthrough curve (Figure 18.2*b*) can be constructed by plotting the relative concentration as a function of time (Robbins, 1983). The relative concentration is $C/C_{\max}$, where $C_{\max}$ is the highest concentration that will be observed at (x,0). $C_{\max}$ is always less than the source concentration C_0.

This breakthrough curve is a cumulative normal distribution with a 2σ value (σ is the standard deviation) that can be derived graphically from Figure 18.2*b* as

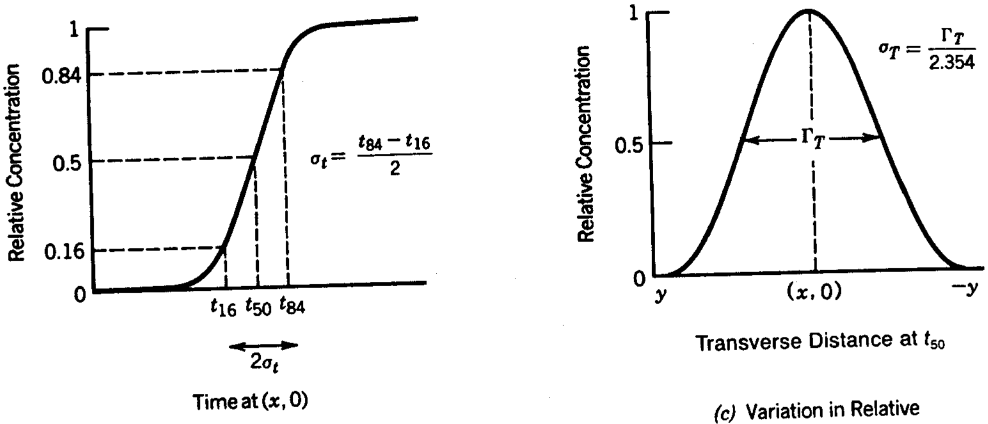
$$2\sigma_t = (t_{84} - t_{16}) \tag{18.1}$$

where t_{84} and t_{16} are the breakthrough times corresponding to relative concentrations of 0.84, and 0.16, respectively. Having calculated σ, the dispersion coefficient is

$$D_L = \frac{v^2\sigma_t^2}{2t} \tag{18.2}$$



(a) Spreading of a Tracer from a point Source



(c) Variation in Relative Concentration along (y, -y)

(b) Breakthrough Curve at (x, 0)

Figure 18.2
Pattern of spreading of a tracer from a continuous point source in a one-dimensional flow field. Two graphical procedures for estimating the standard deviation of a normal distribution are shown in (*b*) and (*c*) (from Robbins, 1983).

The following equation relates the dispersion coefficient to the dispersivity (α) and the linear flow velocity

$$D_L = \alpha_L v \tag{18.3}$$

The same approach can be followed to establish values of dispersivity in the transverse direction. This time the relative concentration is plotted as a function of distance traveled transverse to the direction of flow at t_{50} (Robbins, 1983). The resulting concentration distribution is again normal (Figure 18.2*c*). Once the variance is estimated, the dispersion coefficient is

$$D_T = \frac{\sigma_T^2}{2t} \tag{18.4}$$

The standard deviation in this case (Figure 18.2*c*) is related to the half-width of the distribution (Γ) at a relative concentration of $0.5C_{\max}$ (Robbins, 1983)

$$\sigma_T = \frac{\Gamma}{2.354} \tag{18.5}$$