

Chapter Two

Johnson 1963; Bear 1972; Bear and Verruijt 1987) and the effects of diffusion can be ignored. Under these conditions D_t can be replaced with $\alpha_t v_t$ in the advection-dispersion equations.

Analytical Solutions of the Advection-Dispersion Equation

2.8.1 Methods of Solution

The advection-dispersion equations can be solved by either numerical or analytical methods. Analytical methods involve the solution of the partial differential equations using calculus based on the initial and boundary value conditions. They are limited to simple geometry and in general require that the aquifer be homogeneous. A number of analytical solutions are presented in this chapter. They are useful in that they can be solved with a calculator and a table of error functions or even a pencil and paper, if one is so inclined.

Numerical methods involve the solution of the partial differential equation by numerical methods of analysis. They are more powerful than analytical solutions in the sense that aquifers of any geometry can be analyzed and aquifer heterogeneities can be accommodated. However, there can be other problems with numerical models, such as numerical errors, which can cause solutions to show excess spreading of solute fronts or plumes that are not related to the dispersion of the tracer that is the subject of the modeling. Bear and Verruijt (1987) present a good introduction to the use of numerical models to solve mass transport equations. These solutions are normally found by methods of computer modeling, a topic beyond the scope of this text.

2.8.2 Boundary and Initial Conditions

In order to obtain a unique solution to a differential equation it is necessary to specify the initial and the boundary conditions that apply. The **initial conditions** describe the values of the variable under consideration, in this case concentration, at some initial time equal to 0. The **boundary conditions** specify the interaction between the area under investigation and its external environment.

There are three types of boundary conditions for mass transport. The boundary condition of the first type is a **fixed concentration**. The boundary condition of the second type is a **fixed gradient**. A **variable flux** boundary constitutes the boundary condition of the third type.

Boundary and initial conditions are shown in a shorthand form. For one-dimensional flow we need to specify the conditions relative to the location, x , and the time, t . By convention this is shown in the form

$$C(x, t) = C(t)$$

where $C(t)$ is some known function.

For example, we can write

$$\begin{aligned} C(0, t) &= C_0, & t \geq 0 \\ C(x, 0) &= 0, & x \geq 0 \\ C(\infty, t) &= 0, & t \geq 0 \end{aligned}$$

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The first statement says that for all time t equal to or greater than zero, at $x = 0$ the concentration is maintained at C_0 . This is a fixed-concentration boundary condition located at $x = 0$ (first-type boundary). The second statement is an initial condition that says at time $t = 0$, the concentration is zero everywhere within the flow domain, that is, where x is greater than or equal zero. As soon as flow starts, solute at a concentration of C_0 will cross the $x = 0$ boundary.

The third condition shows that the flow system is infinitely long and that no matter how large time gets, the concentration will still be zero at the end of the system (first-type boundary condition at $x = \infty$).

We could also have specified an initial condition that within the domain the initial solute concentration was C_i . This would be written as

$$C(x, 0) = C_i, \quad x \geq 0$$

Other examples of concentration (first-type) boundary conditions are exponential decay of the source term and pulse loading at a constant concentration for a period of time followed by another period of time with a different constant concentration.

Exponential decay for the source term can be expressed as

$$C(0, t) = C_0 t^{-it}$$

where i = a decay constant.

Pulse loading where the concentration is C_0 for times from 0 to t_0 and then is 0 for all time more than t_0 is expressed as

$$\begin{aligned} C(0, t) &= C_0 & 0 < t \leq t_0 \\ C(0, t) &= 0 & t > t_0 \end{aligned}$$

Fixed-gradient boundaries are expressed as

$$\left. \frac{dC}{dx} \right|_{x=0} = f(t) \quad \text{or} \quad \left. \frac{dC}{dx} \right|_{x=\infty} = f(t)$$

where $f(t)$ is some known function. A common fixed-gradient condition is $dC/dx = 0$, or a no-gradient boundary.

The variable-flux boundary, a third type, is given as

$$-D \frac{\partial C}{\partial x} + v_x C = v_x C(t)$$

where $C(t)$ is a known concentration function. A common variable-flux boundary is a constant flux with a constant input concentration, expressed as

$$\left(-D \frac{dC}{dx} + vC \right) \Big|_{x=0} = vC_0$$

2.8.3 One-Dimensional Step Change in Concentration (First-Type Boundary)

Sand column experiments have been used to evaluate both the coefficients of diffusion and dispersion at the laboratory scale. A tube is filled with sand and then saturated with water. Water is made to flow through the tube at a steady rate, creating, in effect, a permeameter. A solution containing a tracer is then introduced into the sand column

in place of the water. The initial concentration of the solute in the column is zero, and the concentration of the tracer solution is C_0 . The tracer in the water exiting the tube is analyzed, and the ratio of C , the tracer concentration at time t , over C_0 , the injected tracer concentration, is plotted as a function of time. This is called a **fixed-step function**.

The boundary and initial conditions are given by

$$\begin{aligned} C(x, 0) = 0 \quad x \geq 0 & \quad \text{Initial condition} \\ C(0, t) = C_0 \quad t \geq 0 \\ C(\infty, t) = 0 \quad t \geq 0 \end{aligned} \quad \left. \vphantom{\begin{aligned} C(x, 0) = 0 \\ C(0, t) = C_0 \\ C(\infty, t) = 0 \end{aligned}} \right\} \text{Boundary conditions}$$

The solution to Equation 2.18 for these conditions is (Ogata and Banks 1961)

$$C = \frac{C_0}{2} \left[\operatorname{erfc} \left(\frac{L - v_x t}{2\sqrt{D_L t}} \right) + \exp \left(\frac{v_x L}{D_L} \right) \operatorname{erfc} \left(\frac{L + v_x t}{2\sqrt{D_L t}} \right) \right] \quad (2.21)$$

This equation may be expressed in dimensionless form as

$$C_R(t_R, P_e) = 0.5 \left\{ \operatorname{erfc} \left[\left(\frac{P_e}{4t_R} \right)^{1/2} (1 - t_R) \right] + \exp(P_e) \operatorname{erfc} \left[\left(\frac{P_e}{4t_R} \right)^{1/2} (1 + t_R) \right] \right\} \quad (2.22)$$

where

$$t_R = v_x t / L$$

$$C_R = C / C_0$$

$$P_e = \text{Peclet number when flow distance, } L, \text{ is chosen as the reference length} \\ (P_e = v_x L / D_L)$$

erfc = complementary error function

2.8.4 One-Dimensional Continuous Injection into a Flow Field (Second-Type Boundary)

In nature there are not many situations where there would be a sudden change in the quality of the water entering an aquifer. A much more likely condition is that there would be leakage of contaminated water into the ground water flowing in an aquifer. For the one-dimensional case, this might be a canal that is discharging contaminated water into an aquifer as a line source (Figure 2.8).

The rate of injection is considered to be constant, with the injected mass of the solute proportional to the duration of the injection. The initial concentration of the solute in the aquifer is zero, and the concentration of the solute being injected is C_0 . The solute is free to disperse both up-gradient and down-gradient.

The boundary and initial conditions are

$$\begin{aligned} C(x, 0) = 0, \quad -\infty < x < +\infty & \quad \text{Initial condition} \\ \int_{-\infty}^{+\infty} n_s C(x, t) dx = C_0 n_s v_x t, \quad t > 0 \\ C(\infty, t) = 0, \quad t \geq 0 \end{aligned} \quad \left. \vphantom{\begin{aligned} C(x, 0) = 0 \\ \int_{-\infty}^{+\infty} n_s C(x, t) dx = C_0 n_s v_x t \\ C(\infty, t) = 0 \end{aligned}} \right\} \text{Boundary conditions}$$

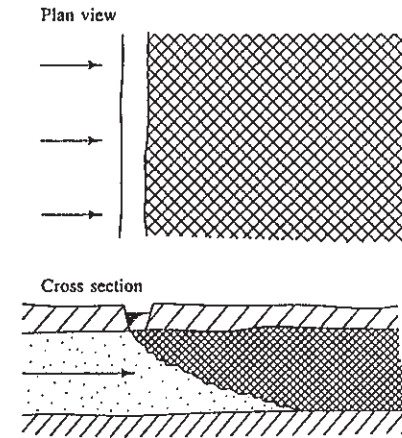


FIGURE 2.8 Leakage from a canal as a line source for injection of a contaminant into an aquifer. Source: J. P. Sauty, *Water Resources Research* 16, no. 1 (1980): 145–58. Copyright by the American Geophysical Union.

The second boundary condition states that the injected mass of contaminant over the domain from $-\infty$ to $+\infty$ is proportional to the length of time of the injection.

The solution to this flow problem (Sauty 1980) is

$$C = \frac{C_0}{2} \left[\operatorname{erfc} \left(\frac{L - v_x t}{2\sqrt{D_L t}} \right) - \exp \left(\frac{v_x L}{D_L} \right) \operatorname{erfc} \left(\frac{L + v_x t}{2\sqrt{D_L t}} \right) \right] \quad (2.23)$$

In dimensionless form this is

$$\begin{aligned} C_R(t_R, P_e) = 0.5 \left\{ \operatorname{erfc} \left[\left(\frac{P_e}{4t_R} \right)^{1/2} (1 - t_R) \right] \right. \\ \left. - \exp(P_e) \operatorname{erfc} \left[\left(\frac{P_e}{4t_R} \right)^{1/2} (1 + t_R) \right] \right\} \end{aligned} \quad (2.24)$$

It can be seen that Equations 2.21 and 2.23 are very similar, the only difference being that the second term is subtracted rather than added in 2.23.

Sauty (1980) gives an approximation for the one-dimensional dispersion equation as

$$C = \frac{C_0}{2} \left[\operatorname{erfc} \left(\frac{L - v_x t}{2\sqrt{D_L t}} \right) \right] \quad (2.25)$$

In dimensionless form this is

$$C_R(t_R, P_e) = 0.5 \operatorname{erfc} \left[\left(\frac{P_e}{4t_R} \right)^{1/2} (1 - t_R) \right] \quad (2.26)$$

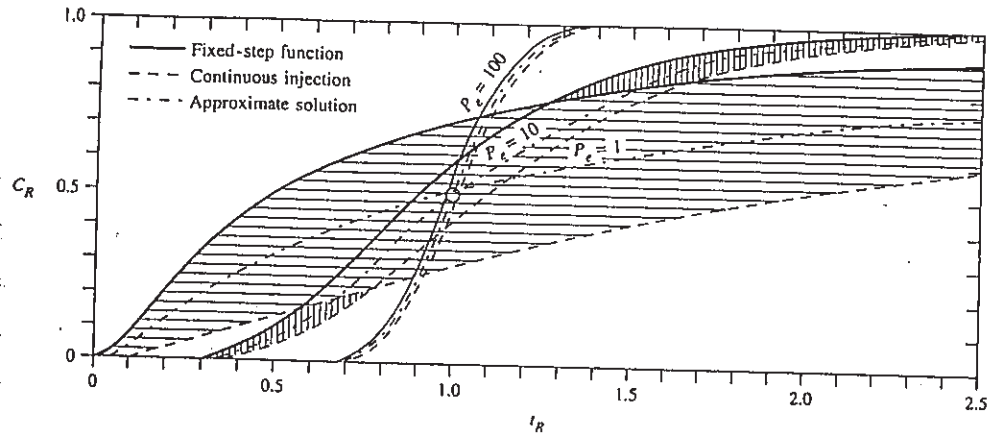


FIGURE 2.9 Dimensionless-type curves for the continuous injection of a tracer into a one-dimensional flow field. Source: J. P. Sauty, *Water Resources Research* 16, no. 1 (1980):145–58. Copyright by the American Geophysical Union.

This approximation comes about because for large Peclet numbers, the second term of Equations 2.21 and 2.23 is much smaller than first term and can be neglected. Figure 2.9 demonstrates under what conditions this approximation is valid. In Figure 2.9 the dimensionless concentration, C_R , is plotted as a function of dimensionless time, t_R , for continuous tracer injection using the fixed-step function, Equation 2.22, the continuous-injection function, Equation 2.24, and the approximate solution, Equation 2.26. Curves are plotted for three Peclet numbers, 1, 10, and 100. Sauty (1980) defined a Peclet number as $P_e = v_x L / D_L$, where L is the distance from the point of injection of the solute to the point of measurement and D_L is the coefficient of hydrodynamic dispersion. This Peclet number defines the rate of transport by advection to the rate of transport by hydrodynamic dispersion. For Peclet number 1, the fixed-step function and the continuous-injection function give quite different results, whereas for Peclet number 100 they are almost identical. The approximate solution lies midway between the other two. This figure suggests that for Peclet numbers less than about 10, the exact solutions need to be considered, whereas for Peclet numbers greater than 10, the approximate solution is probably acceptable, especially as the Peclet number approaches 100. This Peclet number increases with flow-path length as advective transport becomes more dominant over dispersive transport. Thus for mass transport near the inlet boundary, it is important to use the correct equation, but as one goes away from the inlet boundary, it is less important that the correct form of the equation is employed.

2.8.5 Third-Type Boundary Condition

A solution for Equation 2.18 for the following boundary condition was given by van Genuchten (1981).

$$\left. \begin{aligned} C(x, 0) &= 0 && \text{Initial condition} \\ \left(-D \frac{\partial C}{\partial x} + v_x C \right) \Big|_{x=0} &= v_x C_0 \\ \frac{\partial C}{\partial x} \Big|_{x \rightarrow \infty} &= (\text{finite}) \end{aligned} \right\} \text{Boundary conditions}$$

The third condition specifies that as x approaches infinity, the concentration gradient will still be finite. Under these conditions the solution to Equation 2.18 is:

$$C = \frac{C_0}{2} \left[\operatorname{erfc} \left[\frac{L - v_x t}{2\sqrt{D_L t}} \right] + \left(\frac{v_x^2 t}{\pi D_L} \right)^{1/2} \exp \left[-\frac{(L - v_x t)^2}{4D_L t} \right] - \frac{1}{2} \left(1 + \frac{v_x L}{D_L} + \frac{v_x^2 t}{D_L} \right) \exp \left(\frac{v_x L}{D_L} \right) \operatorname{erfc} \left[\frac{L - v_x t}{2\sqrt{D_L t}} \right] \right] \quad (2.27)$$

This equation also reduces to the approximate solution, Equation 2.25, as the flow length increases.

2.8.6 One-Dimensional Slug Injection into a Flow Field

If a slug of contamination is instantaneously injected into a uniform, one-dimensional flow field, it will pass through the aquifer as a pulse with a peak concentration, C_{max} , at some time after injection, t_{max} . The solution to Equation 2.18 under these conditions (Sauty 1980) is in dimensionless form:

$$C_R(t_R, P_e) = \frac{E}{(t_R)^{1/2}} \exp \left(-\frac{P_e}{4t_R} (1 - t_R)^2 \right) \quad (2.28)$$

with

$$E = (t_{Rmax})^{1/2} \cdot \exp \left(\frac{P_e}{4t_{Rmax}} (1 - t_{Rmax})^2 \right) \quad (2.29)$$

where

$$t_{Rmax} = (1 + P_e^{-2})^{1/2} - P_e^{-1} \text{ (dimensionless time at which peak concentration occurs)}$$

$$C_R = C / C_{max}$$

In Figure 2.10, $C_R (C/C_{max})$ for a slug injected into a uniform one-dimensional flow field is plotted against dimensionless time, t_R , for several Peclet numbers. It can be seen that the time for the peak concentration (C_{max}) to occur increases with the Peclet number, up to a limit of $t_R = 1$. Breakthrough becomes more symmetric with increasing P_e .

2.8.7 Continuous Injection into a Uniform Two-Dimensional Flow Field

If a tracer is continuously injected into a uniform flow field from a single point that fully penetrates the aquifer, a two-dimensional plume will form that looks similar to Figure

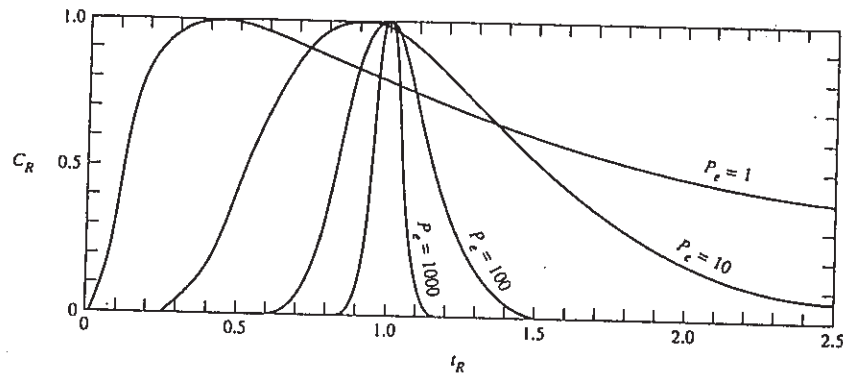


FIGURE 2.10 Dimensionless-type curve for the injection of a slug of a tracer into a one-dimensional flow field. Source: J. P. Sauly, *Water Resources Research* 16, no. 1 (1980):145-58. Copyright by the American Geophysical Union.

2.11. It will spread along the axis of flow due to longitudinal dispersion and normal to the axis of flow due to transverse dispersion. This is the type of contamination that would occur due to leakage of liquids from a landfill or lagoon.

The mass transport equation for two-dimensional flow, Equation 2.19, has been solved for several boundary conditions. The well is located at the origin ($x = 0, y = 0$) and there is a uniform velocity at a rate v_x parallel to the x axis. There is a continuous injection of a solute of concentration, C_0 , at a rate Q at the origin.

Bear (1972) gives the solution to Equation 2.19 for the condition where the growth of the plume has stabilized—that is, as time approaches infinity—as

$$C(x, y) = \left(\frac{C_0 Q}{2\pi(D_L D_T)^{1/2}} \right) \exp\left(\frac{v_x x}{2D_L D_T} \right) K_0 \left[\left(\frac{v_x^2}{4D_L} \left(\frac{x^2}{D_L} + \frac{y^2}{D_T} \right) \right)^{1/2} \right] \quad (2.30)$$

where

K_0 = the modified Bessel function of the second kind and zero order (values are tabulated in Appendix B)

Q = rate at which a tracer of concentration C_0 is being injected

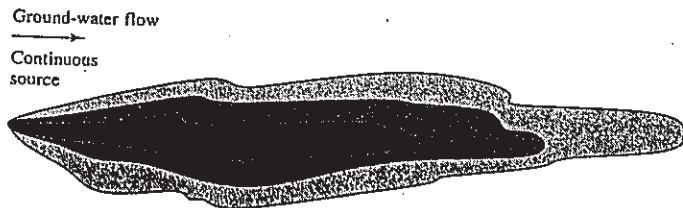


FIGURE 2.11 Plume resulting from the continuous injection of a tracer into a two-dimensional flow field. Source: C. W. Fetter, *Applied Hydrogeology*, 2nd ed. (New York: Macmillan Publishing Company, 1988).

The two-dimensional growth of a plume from a continuous source can be tracked through time using a solution to Equation 2.19 developed by Y. Emsellem (see Fried 1975). The solution has the form

$$C(x, y, t) = \frac{C_0 Q}{4\pi(D_L D_T)^{1/2}} \exp\left(\frac{v_x x}{2D_L} \right) [W(0, B) - W(t, B)] \quad (2.31)$$

where

$$B = \left[\frac{(v_x x)^2}{4D_L^2} + \frac{(v_x y)^2}{4D_L D_T} \right]^{1/2}$$

t = time

$W[t, B]$ = a function derived by Hantush and tabulated in Appendix C (In well hydraulics this function is known as the leaky well function $W[u, r/b]$.)

2.8.8 Slug Injection into a Uniform Two-Dimensional Flow Field

If a slug of contamination is injected over the full thickness of a two-dimensional uniform flow field in a short period of time, it will move in the direction of flow and spread with time. This result is illustrated by Figure 2.12 and represents the pattern of contamination at three increments that result from a one-time spill. Figure 2.12 is based on the results of a laboratory experiment conducted by Bear (1961). Figure 2.13 shows the spread of a plume of chloride that was injected into an aquifer as a part of a large-scale field test (Mackay et al. 1986). The plume that resulted from the field test is more complex than the laboratory plume due to the heterogeneities encountered in the real world and the fact the plume may not be following the diffusional model of dispersion.

De Josselin De Jong (1958) derived a solution to this problem on the basis of a statistical treatment of lateral and transverse dispersivities. Bear (1961) later verified it experimentally. If a tracer with concentration C_0 is injected into a two-dimensional flow field over an area A at a point (x_0, y_0) , the concentration at a point (x, y) , at time t after the injection is

$$C(x, y, t) = \frac{C_0 A}{4\pi t(D_L D_T)^{1/2}} \exp\left[-\frac{(x - (x_0 - v_x t))^2}{4D_L t} - \frac{(y - y_0)^2}{4D_T t} \right] \quad (2.32)$$

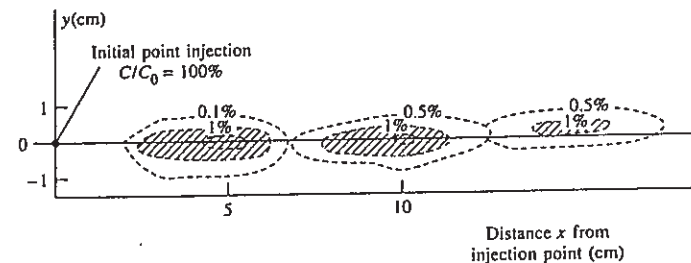


FIGURE 2.12 Injection of a slug of a tracer into a two-dimensional flow field shown at three time increments. Experimental results from J. Bear, *Journal of Geophysical Research* 66, no. 8 (1961):2455-67. Copyright by the American Geophysical Union.

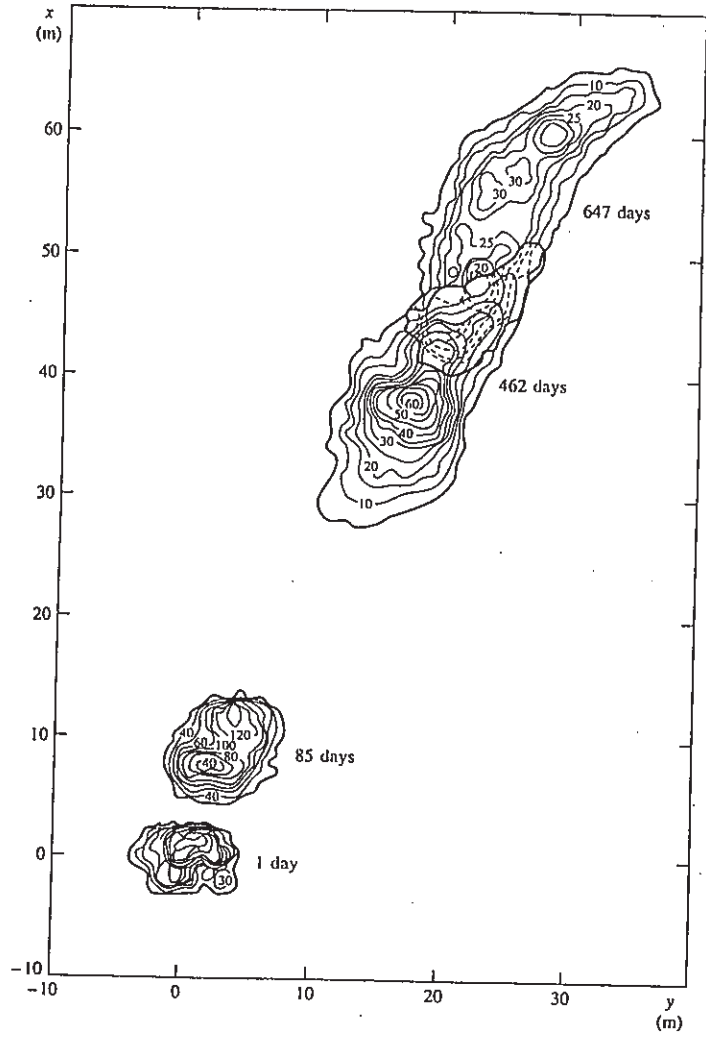


FIGURE 2.13 Vertically averaged chloride concentration at 1 day, 85 days, 462 days, and 647 days after the injection of a slug into a shallow aquifer. Source: D. M. Mackay et al. *Water Resources Research* 22, no. 13 (1986):2017–29. Copyright by the American Geophysical Union.