

# 1

## Darcy's Law and Advective Transport

### 1.1 AVERAGE PARTICLE VELOCITY AND TIME OF TRAVEL

Figure 1-1 shows a pipe, one section of which is packed with sand; water of uniform density and viscosity flows through the pipe under pressure, so that the pipe remains full and the sand remains saturated. The rate of flow, in volume of water per unit time, is designated  $Q$ . Piezometers at either end of the sand section are used to measure the hydraulic head,  $h$ , or elevation of the piezometric water level above datum; the cross-sectional area of the pipe is designated  $A$ , and the length of the sand section as  $L$ . The flow rate through the sand section is given by

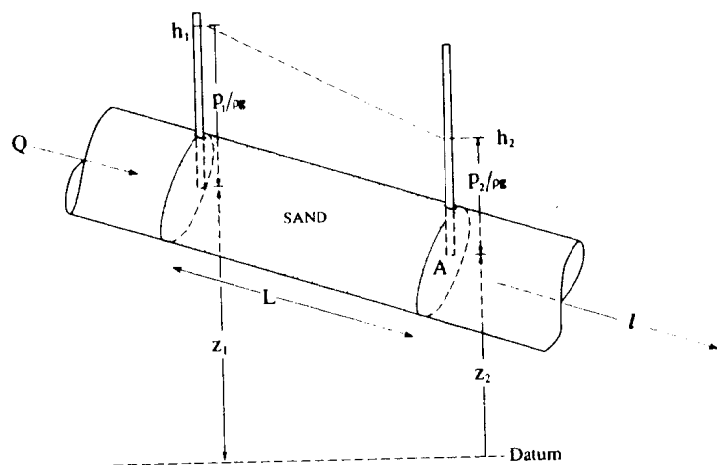
$$Q = -KA \frac{h_2 - h_1}{L} \quad (1-1)$$

where  $K$  is the hydraulic conductivity of the sand;  $h_1$  the head at the upstream face and  $h_2$  the head at the downstream face. Equation (1-1) is a form of Darcy's Law, the fundamental relation describing flow in porous media (Darcy, 1856).

Expressed in terms of the derivative or gradient of head, Darcy's law for the problem of Figure 1-1 may be written as

$$Q = -KA \frac{dh}{dl} \quad (1-2)$$

where  $l$  represents distance along the pipe.

FIGURE 1-1. Sand-packed pipe section carrying a flow  $Q$ .

The head,  $h$ , measures the potential energy of a unit weight of water located at the point of measurement. Within the sand section, the loss of head between two points represents the energy or work required to move a unit weight of water between those points. Note that the head, at points within the sand, has two components, i.e.,

$$h = z + \frac{P}{\rho g} \quad (1-3)$$

where  $z$  is the elevation of the point above datum;  $P$  the pressure;  $\rho$  the mass density of the water;  $g$  the acceleration of gravity; and the term  $P/(\rho g)$  is the height to which water will rise in a piezometer open at that point. Readers familiar with open flow hydraulics will note that the kinetic term  $v^2/(2g)$ , where  $v$  is the water velocity, is not included in equation (1-3). Velocities of flow within a porous medium are normally low enough so that this term is negligible. Darcy's Law can be stated in much more general terms (see Section 1.2), but equations (1-1) or (1-2) are adequate to describe the flow regime in the system of Figure 1-1.

Now suppose we are interested not just in the quantity of flow passing through the sand, but in the time it takes water to pass from one face of the sand section to the other. We begin by assuming that there may be some fraction of the pore space in which velocity is zero, i.e., in which the water

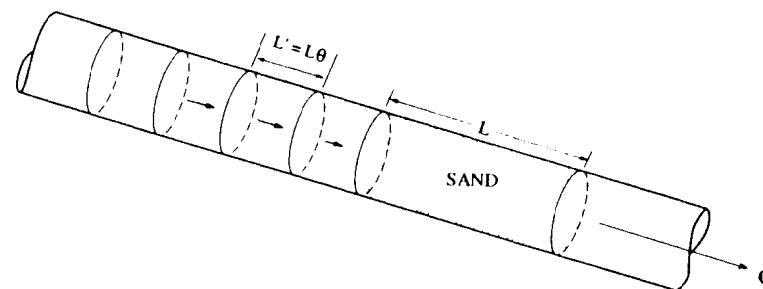


FIGURE 1-2. Pipe of Figure 1-1, showing a series of pore volumes approaching the sand section.

is completely static; examples might include "dead-end" pore space or fully isolated pores. We use the term *effective porosity* to designate the ratio of the remaining pore volume, i.e., that containing moving water, to the bulk volume of the sand. To simplify the analysis we assume initially that the velocity is completely uniform throughout this segment of the pore space. Under this assumption, the water in the sand which is free to move is totally displaced, in a certain time interval, by new water entering through the upstream sand face. The volume of moving water within the sand at any time is  $\theta AL$ , where  $\theta$  is the effective porosity. For purposes of travel time calculation, we consider the quantity  $\theta AL$  to be a "pore volume," since it represents the volume of pore space in which flow occurs. We can think of the flow as a succession of discrete pore volumes moving along the pipe as shown in Figure 1-2, so that each pore volume is displaced from the sand in turn by the following pore volume. (Note that before entering the sand, or after leaving it, each pore volume occupies a distance  $L'$  along the pipe, where  $L' = L\theta$ .)

The displacement of a pore volume from the sand requires a certain time interval,  $\Delta t_p$ ; and by definition, the displaced liquid volume divided by this time interval is the flow rate,  $Q$ , i.e.

$$Q = \frac{\theta AL}{\Delta t_p} \quad (1-4)$$

or

$$\Delta t_p = \frac{\theta AL}{Q} \quad (1-5)$$

If we consider the successive pore volumes in Figure 1-2 to be separated by liquid interfaces,  $\Delta t_p$  is obviously the time required for one of these

interfaces to move completely through the sand section; thus  $\Delta t_p$  can be interpreted as the time required for a fluid particle to traverse the distance  $L$  within the sand. More generally, if flow at a rate  $Q$  occurs through a given volume of aquifer  $V$ , the term  $\theta V/Q$  gives the time required for movement of a fluid interface through the volume  $V$  along the path of flow.

We can define an average seepage velocity, or, interstitial velocity,  $v$ , through the sand section of Figure 1-2, as  $L/\Delta t_p$ , i.e.,

$$v = \frac{L}{\Delta t_p} = \frac{Q}{\theta A} \quad (1-6)$$

Substituting equation (1-2) into the above equation yields

$$v = -\frac{K}{\theta} \frac{dh}{dl} \quad (1-7)$$

In writing Darcy's Law, we frequently use the Darcy velocity,  $q$  or  $Q/A$ , i.e.,

$$q = \frac{Q}{A} = -K \frac{dh}{dl} \quad (1-8)$$

and it is important to distinguish this Darcy velocity from the seepage velocity defined in equation (1-6) or (1-7). The Darcy velocity is actually a discharge per unit bulk area of sand face, and is often referred to as specific discharge; it represents the average fluid velocity in the open pipe, outside the sand section in Figure 1-2, but is less than the seepage velocity within the sand by the factor  $\theta$ . To view this in another way, the cross-sectional area of flow in the sand ( $\theta A$ ) is smaller than that in the open pipe ( $A$ ); and since the same discharge prevails in each section, velocity must be greater within the sand.

It should also be noted that even under our assumption that velocity is uniform within the effective component of the pore space, the seepage velocity,  $v$ , is not the true velocity of movement within the sand. Any fluid particle moving through the sand section must travel a greater distance than  $L$ , since the flow path must necessarily involve tortuous movement around the sand grains. Thus the actual particle velocity must exceed  $L/\Delta t_p$ . The seepage velocity, however, gives the apparent velocity in terms of linear distance along the exterior of the porous medium; in field or laboratory problems, this is the quantity which can be measured or calculated.

Before leaving this discussion we note that the flow distribution within the pore space is never actually as simple as that assumed above. Clearly

there is never a perfectly uniform flow velocity throughout one part of the pore space, and zero velocity in the remainder, as assumed in the preceding development; and in fact the role of porosity in solute transport is far more complex than this example would suggest. However, where an independent measure of *total porosity* (the ratio of total pore volume to bulk volume) is available, one often finds that use of this total porosity in equation (1-5) will yield a travel time which differs from the results of tracer experiments, and that some smaller porosity figure must be used to achieve agreement. This value is taken as the *effective porosity*. As we will see in the following chapter, flow velocities in the pore space actually vary through a wide spectrum; and in the displacement of a "pore volume" of liquid (as measured by the effective porosity) the interstitial water in some parts of the pore space may be replaced several times, while that in other parts of the pore space is only partially replaced, or is not replaced at all. Thus the term *effective porosity*, as used above, should properly be viewed as the porosity required to achieve agreement with observation in a calculation of travel time. Where seepage velocity can be estimated from the observed travel time of a tracer, effective porosity is taken as the ratio of Darcy velocity to the measured seepage velocity. This interpretation has numerous implications which can be considered more fully as our discussion of general solute transport processes is developed; further discussion of porosity in solute transport calculation is therefore deferred to Chapter 2. Unless otherwise indicated, however, the term *porosity* and the symbol  $\theta$ , as used in this text, refer to effective porosity in the sense used above.

To return to the relationship between time of flow, volume of liquid and flow rate, the pipe in Figure 1-2 is analogous to a stream tube in steady-state groundwater flow, i.e., a region in a flow field which is bounded by a stream surface, or surface across which no flow occurs. If a system of stream tubes can be defined in a steady-state flow field, times of travel can readily be estimated. As in the example of Figure 1-2, this is done by dividing the volumes of water displaced in a section of the stream tube by the flow rate through the stream tube. (For a more detailed discussion of stream tubes or stream functions, see Appendix A).

## 1.2 GENERALIZATION OF DARCY'S LAW AND EQUATION OF GROUNDWATER FLOW

In field problems the Darcy velocity and seepage velocity are generally not unidirectional, as they are in the example in Figure 1-1; thus the simple formulations of equation (1-8) for Darcy's Law and equation (1-7) for the seepage velocity are usually not adequate. This section presents two

formulations of Darcy's Law which can be applied to a wide range of three-dimensional flow problems. More detailed discussions of Darcy's Law are available in standard groundwater texts (e.g., Freeze and Cherry, 1979; Domenico and Schwartz, 1990).

In a three-dimensional problem the Darcy velocity is expressed as a vector through the relation:

$$\mathbf{q} = q_x \mathbf{i} + q_y \mathbf{j} + q_z \mathbf{k} \quad (1-9)$$

where  $\mathbf{q}$  is the Darcy velocity vector;  $\mathbf{i}$ ,  $\mathbf{j}$ , and  $\mathbf{k}$  are the conventional unit vectors in the  $x$ ,  $y$ , and  $z$  coordinate directions; and  $q_x$ ,  $q_y$ , and  $q_z$  are the scalar components of the Darcy velocity in those directions. If the porous medium is characterized by three principal axes of hydraulic conductivity, and if these principal axes are aligned with the coordinate axes, the Darcy velocity components in water of uniform density and viscosity are given by

$$q_x = -K_x \frac{\partial h}{\partial x} \quad (1-10)$$

$$q_y = -K_y \frac{\partial h}{\partial y} \quad (1-11)$$

$$q_z = -K_z \frac{\partial h}{\partial z} \quad (1-12)$$

where  $K_x$ ,  $K_y$ , and  $K_z$  represent the components of hydraulic conductivity in the respective coordinate directions. If the water is not of uniform density and viscosity, the equations are usually formulated in terms of intrinsic permeabilities and pressure gradients, i.e.,

$$q_x = -\frac{k_x}{\mu} \frac{\partial P}{\partial x} \quad (1-13)$$

$$q_y = -\frac{k_y}{\mu} \frac{\partial P}{\partial y} \quad (1-14)$$

$$q_z = -\frac{k_z}{\mu} \left( \frac{\partial P}{\partial z} + \rho g \right) \quad (1-15)$$

where  $P$  is pressure;  $\mu$  is the dynamic viscosity of the water;  $\rho$  is water density;  $k_x$ ,  $k_y$ , and  $k_z$  represent the intrinsic permeabilities in the respective coordinate directions;  $g$  is the acceleration of gravity, which is considered a positive scalar in equation (1-15); and  $z$  is the vertical coordinate, taken

positive upwards. Intrinsic permeability is a function only of the porous medium, whereas hydraulic conductivity incorporates properties of the fluid as well. The two are related by

$$K_x = \frac{k_x \rho g}{\mu} \quad (1-16)$$

for the  $x$  direction, and by similar expressions for the  $y$  and  $z$  directions. Because of the relation between hydraulic head,  $h$ , and pressure,  $P$ , as given in equation (1-3), equations (1-13) through (1-15) specialize to equations (1-10) through (1-12) when density and viscosity are independent of the spatial coordinates.

It should be noted that the hydraulic conductivity or intrinsic permeability is actually a second-rank tensor. If the principal components of hydraulic conductivity or intrinsic permeability are not aligned with horizontal and vertical coordinate axes, velocity components in each direction are a function of head or pressure gradients in all three directions, rather than solely in the direction of the velocity component. Thus, in terms of head, equations (1-10) through (1-12) must be written as

$$q_x = -K_{xx} \frac{\partial h}{\partial x} - K_{xy} \frac{\partial h}{\partial y} - K_{xz} \frac{\partial h}{\partial z} \quad (1-17)$$

$$q_y = -K_{yx} \frac{\partial h}{\partial x} - K_{yy} \frac{\partial h}{\partial y} - K_{yz} \frac{\partial h}{\partial z} \quad (1-18)$$

$$q_z = -K_{zx} \frac{\partial h}{\partial x} - K_{zy} \frac{\partial h}{\partial y} - K_{zz} \frac{\partial h}{\partial z} \quad (1-19)$$

where  $K_{xx}$ ,  $K_{yy}$ , and  $K_{zz}$  are principal components of the hydraulic conductivity tensor, while  $K_{xy}$ ,  $K_{xz}$ ,  $K_{yx}$ ,  $K_{yz}$ ,  $K_{zx}$ , and  $K_{zy}$  are cross terms of that tensor. In practical applications, equations (1-17) through (1-19) are rarely used. In other words, it is generally assumed that the principal components of the hydraulic conductivity tensor can be aligned with horizontal and vertical coordinate axes so that the cross terms of the hydraulic conductivity tensor become zero.

When the Darcy velocity is calculated as a vector point function using equation (1-9), the average seepage velocity is also taken as a vector point function, and is simply the Darcy velocity vector divided by the (scalar) effective porosity, i.e.,

$$\mathbf{v} = \frac{\mathbf{q}}{\theta} = \frac{q_x}{\theta} \mathbf{i} + \frac{q_y}{\theta} \mathbf{j} + \frac{q_z}{\theta} \mathbf{k} \quad (1-20)$$

or

$$\begin{aligned}v_x &= q_x/\theta \\v_y &= q_y/\theta \\v_z &= q_z/\theta\end{aligned}\quad (1-21)$$

The seepage velocity components in equation (1-21) are obtained by first solving the differential equation of groundwater flow to obtain head or pressure as a function of the spatial coordinates and time; then invoking equations (1-10) through (1-12) or (1-13) through (1-15) to calculate Darcy velocity components throughout the region and time span of interest; and finally converting the Darcy velocity terms to seepage velocities using the porosity. In terms of head, which is the most convenient formulation if the water is of uniform density and viscosity, the differential equation of groundwater flow takes the form (see for example Freeze and Cherry, 1979; Domenico and Schwartz, 1990):

$$\frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) + q_s = S_s \frac{\partial h}{\partial t} \quad (1-22)$$

where  $q_s$  is the fluid sink/source term, or volumetric rate at which water is added to or removed from the system per unit volume of aquifer;  $S_s$  is the specific storage, or volume of water released from storage in a unit volume of aquifer per unit decline in head; and it is assumed that the aquifer is characterized by three orthogonal principal directions of hydraulic conductivity, with which the coordinate axes are aligned.

If viscosity and density are not uniform, the flow equation is more conveniently formulated in terms of pressure. We again assume three orthogonal coordinate axes, but now add the condition that the  $z$  axis is along the vertical. We also assume that spatial variations in density are due primarily to changes in solute concentration, and that spatial differences in the mass of pure water per unit volume due to variations of pressure are negligible in comparison. Under these assumptions, letting  $z$  represent the vertical direction and taking  $z$  positive upward, the equation of flow can be written as

$$\frac{\partial}{\partial x} \left( \frac{k_x}{\mu} \frac{\partial P}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{k_y}{\mu} \frac{\partial P}{\partial y} \right) + \frac{\partial}{\partial z} \left\{ \frac{k_z}{\mu} \left( \frac{\partial P}{\partial z} + \rho g \right) \right\} + q_s = S_{sp} \frac{\partial P}{\partial t} \quad (1-23)$$

where  $S_{sp}$  is the specific storage in terms of pressure, or the volume of water released from storage in a unit volume of aquifer in response to a unit decline in pressure.

### 1.3 ADVECTIVE TRANSPORT

Section 1.1 considered the average rate of movement and time of travel of fluid particles. So long as the fluid particles in a groundwater regime are chemically and physically indistinguishable, there is little reason to be concerned with these topics. Frequently, however, the fluid particles are not all identical. Some particles, although fully miscible with the groundwater, may be "tagged"—they may represent a dissolved tracer, or water of higher salinity, or a dissolved organic contaminant. The movement of such "tagged" particles is termed solute transport; in this section we will derive equations of solute transport under the simplifying assumption of Section 1.1, that all solute particles move with the average seepage velocity of the water. Equations of this type are termed advective transport equations; equations of transport which incorporate other processes are developed in Chapters 2 and 3.

#### 1.3.1 Mass-Balance Considerations and the Eulerian Approach to Advective Transport

We will first develop the equation of advective transport through a mass-balance approach. This approach requires that the concentration of the solute be introduced as the primary dependent variable. Suppose that the water moving through the sand of Figure 1-2 contains dissolved salt or tracer at a concentration  $C$ , in units of mass of solute per volume of water. The mass of solute transported across a plane at right angles to the pipe in the sand-packed section of Figure 1-2 is given by

$$Q_m = QC \quad (1-24)$$

where  $Q_m$  is the mass of solute crossing the plane per unit time and  $Q$  is again the volumetric fluid discharge (volume per unit time) through the sand. Using the Darcy velocity vector,  $\mathbf{q}$ , as in equation (1-9), rather than the fluid discharge,  $Q$ , an advective mass flux vector may be calculated as

$$\mathbf{q}_m = \mathbf{q}C \quad (1-25)$$

where  $\mathbf{q}_m$  is a vector having the direction of the Darcy velocity and a magnitude equal to the mass of solute transported advectively per unit time across a unit area normal to the flow.

Figure 1-3 shows the apparatus of Figures 1-1 and 1-2 again, but now showing two cross-sectional planes, each normal to the flow and separated by a distance  $\Delta l$ ; thus the two planes enclose a bulk volume  $A \Delta l$ , where  $A$

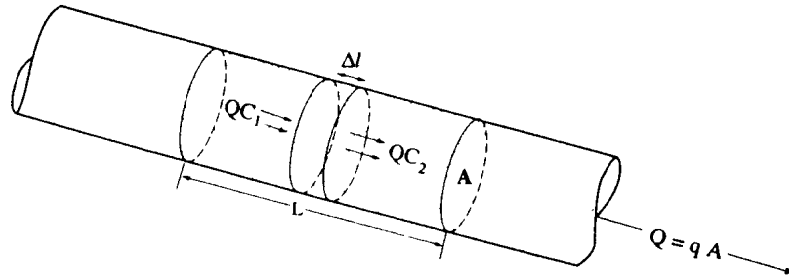


FIGURE 1-3. Pipe of Figure 1-1, showing solute mass transport into and out of a volume element.

is again the cross-sectional area of the pipe. Let us suppose that the concentration of salt or tracer in the water moving through the system varies along the pipe (but is constant over any cross-sectional plane normal to the pipe). At the upstream cross section of Figure 1-3 we designate the concentration  $C_1$ , and at the downstream cross section,  $C_2$ . The rate at which solute mass enters the volume  $A \Delta l$  at the upstream face,  $Q_{m1}$ , is then equal to  $QC_1$ ; the rate at which it leaves that volume at the downstream face,  $Q_{m2}$ , is given by  $QC_2$ . Because these two rates differ, the mass of solute within the volume  $A \Delta l$  must change with time, at a rate equal to the difference between the rates of mass inflow and mass outflow. Letting  $M$  represent the mass of solute in the volume  $A \Delta l$ , and  $dM/dt$  the rate at which that mass changes with time,

$$\frac{dM}{dt} = QC_1 - QC_2 \quad (1-26)$$

or equivalently

$$\frac{dM}{dt} = qA(C_1 - C_2) \quad (1-27)$$

where  $q$  is the scalar magnitude of the Darcy velocity.

To simplify the analysis we assume that the solute carried in advective transport remains completely within the moving water, i.e., that there is no diffusion of solute into and from sections of the pore space which may contain static or nearly static water. In effect, we are assuming that the diffusion of solute into essentially static water (for example, along the pore walls or in dead-end pores) can be neglected, or will be addressed through some separate aspect of the analysis as discussed in the following chapter. Under this assumption, the volume of water containing solute in the bulk volume  $A \Delta l$

is  $\theta A \Delta l$ , where again  $\theta$  is effective porosity; and letting  $C$  represent the average concentration in this volume, the mass of solute between the two planes at any time is given by  $\theta A \Delta l C$ . Thus the rate at which this solute mass changes with time can be expressed in terms of the rate at which concentration changes with time as

$$\frac{dM}{dt} = \theta A \Delta l \frac{\partial C}{\partial t} \quad (1-28)$$

Equating the expressions for  $dM/dt$  in (1-27) and (1-28) gives

$$qA(C_1 - C_2) = \theta A \Delta l \frac{\partial C}{\partial t} \quad (1-29)$$

The concentration difference,  $C_1 - C_2$  can be expressed in terms of the concentration gradient along the pipe,  $\partial C/\partial l$ , as

$$C_1 - C_2 = -\frac{\partial C}{\partial l} \Delta l \quad (1-30)$$

where  $l$  is taken positive in the direction of flow. Combining equations (1-29) and (1-30) gives

$$-qA \frac{\partial C}{\partial l} \Delta l = \theta A \Delta l \frac{\partial C}{\partial t} \quad (1-31)$$

or

$$-q \frac{\partial C}{\partial l} = \theta \frac{\partial C}{\partial t} \quad (1-32)$$

In a more general case we could allow for the possibility that the Darcy velocity itself might vary between the upstream and downstream faces in Figure 1-3. This would imply that the mass of water within the volume  $A \Delta l$  was itself changing, due to elastic storage effects analogous to those observed in confined groundwater systems. Let us assume for simplicity that these storage effects involve no appreciable change in the volume  $A \Delta l$ , i.e., that the storage effects are due only to changes in the density of the water, in response to pressure change, within a rigid porous framework. Under this assumption equation (1-32) can be generalized as

$$-\frac{\partial(qC)}{\partial l} = \theta \frac{\partial C}{\partial t} \quad (1-33)$$

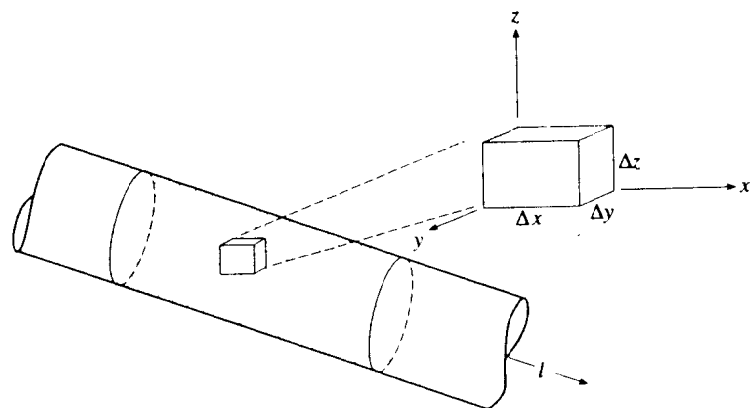


FIGURE 1-4. Volume element for development of the advective transport equation in Cartesian coordinates.

where the change in the product ( $qC$ ) between the faces of the volume element is now recognized as the factor controlling solute accumulation.

An equation for advective transport under more general conditions can be obtained by considering a small volume element within the sand of Figure 1-1 which is not aligned in any way with the flow direction but rather is oriented along a conventional vertical/horizontal Cartesian coordinate system. Figure 1-4 shows this volume element,  $\Delta x \Delta y \Delta z$ . None of the three coordinate axes is either parallel to or normal to the pipe; thus the Darcy velocity vector,  $q$ , has components in all three coordinate directions, and the solute concentration similarly varies in all three directions. For simplicity, we again assume that storage effects involve only changes in fluid density within a rigid porous framework. The cross-sectional area of the element normal to the  $x$  direction is  $\Delta y \Delta z$ ; applying the concepts used in developing equation (1-33), the net inflow minus outflow of solute mass in the  $x$  direction for the volume element is given by

$$-\frac{\partial}{\partial x} (q_x C) \Delta x \Delta y \Delta z \quad (1-34)$$

where  $q_x$  is the component of the Darcy velocity in the  $x$  direction. Similar expressions can be written for the  $y$  and  $z$  directions, so that the total net inflow minus outflow of solute mass for the element is

$$-\left[ \frac{\partial}{\partial x} (q_x C) + \frac{\partial}{\partial y} (q_y C) + \frac{\partial}{\partial z} (q_z C) \right] \Delta x \Delta y \Delta z \quad (1-35)$$

If the volume element of Figure 1-4 contains a fluid source through which water enters the flow regime, or a fluid sink through which water is withdrawn, an additional term is required in the expression for inflow minus outflow. Let  $Q_s$  represent the volumetric rate at which water is added or removed, where a positive sign indicates a source and a negative sign a sink, and let  $C_s$  represent the concentration of solute in the water which is added or withdrawn. The term  $Q_s C_s$  thus represents the net rate at which solute mass is added to or removed from the volume element by the source or sink, expressed in dimensions of mass per unit time. This term must be added to equation (1-35), which represents inflow minus outflow for the volume element, giving

$$-\left[ \frac{\partial}{\partial x} (q_x C) + \frac{\partial}{\partial y} (q_y C) + \frac{\partial}{\partial z} (q_z C) \right] \Delta x \Delta y \Delta z + Q_s C_s \quad (1-36)$$

The rate of accumulation of solute mass within the element is given by  $\theta \Delta x \Delta y \Delta z \partial C / \partial t$ . Equating this rate of accumulation to the expression in (1-36) gives

$$-\frac{\partial}{\partial x} (q_x C) - \frac{\partial}{\partial y} (q_y C) - \frac{\partial}{\partial z} (q_z C) + \frac{Q_s C_s}{\Delta x \Delta y \Delta z} = \theta \frac{\partial C}{\partial t} \quad (1-37)$$

where again it is assumed that any change in the volume of water within the element  $\Delta x \Delta y \Delta z$  can be neglected. Equation (1-37) can be divided by porosity, converting the Darcy velocity components to seepage velocity components,  $v_x$ ,  $v_y$ , and  $v_z$ . This yields the alternative form:

$$-\frac{\partial}{\partial x} (v_x C) - \frac{\partial}{\partial y} (v_y C) - \frac{\partial}{\partial z} (v_z C) + \frac{q_s C_s}{\theta} = \frac{\partial C}{\partial t} \quad (1-38)$$

where  $q_s = Q_s / (\Delta x \Delta y \Delta z)$  is the volumetric inflow rate per unit volume of the aquifer due to the source or sink. Equation (1-38) can also be written in vector form as

$$-\nabla \cdot (vC) + \frac{q_s}{\theta} C_s = \frac{\partial C}{\partial t} \quad (1-39)$$

or in subscript form as

$$-\frac{\partial}{\partial x_i} (v_i C) + \frac{q_s}{\theta} C_s = \frac{\partial C}{\partial t} \quad (1-40)$$

where the subscript  $i$  designates coordinate direction, and summation over all coordinate directions is implied by the notation.

Equations (1-38) through (1-40) provide a more general description of advective transport, suitable for use where the velocity and the concentration vary in three dimensions, and where fluid sinks or sources are present. As the development shows, these forms of the equation are required even where the velocity and the concentration gradient are unidirectional and colinear, if the coordinate system is not itself aligned with the direction of flow.

The development of equations (1-37) through (1-40) is based on the assumption of a rigid aquifer, i.e., the assumption that changes in the quantity of water in storage are due only to expansion or compression of the interstitial water. Confined storage is normally attributed both to changes in water density and to deformation of the aquifer (e.g., Cooper, 1966). Exact analysis of the solute mass balance in a deforming aquifer is considerably more complex than that for a rigid aquifer. If it is assumed that the aquifer is deforming, allowance must be made for the fact that the porosity,  $\theta$ , must change with time. Thus in developing a solute mass balance for a fixed spatial volume element, porosity should appear under the time derivative in the expression for rate of solute mass accumulation. For example, in developing equation (1-37), the rate of solute mass accumulation within the element  $\Delta x \Delta y \Delta z$  should be taken as  $\partial(\theta C)/\partial t \Delta x \Delta y \Delta z$  rather than as  $\theta \partial C/\partial t \Delta x \Delta y \Delta z$ . This would lead to an exact solution for solute mass balance if the specific discharge terms on the left-hand side of equation (1-37),  $q_x$ ,  $q_y$ , and  $q_z$ , represented the true liquid fluxes across the faces of the element in a deforming aquifer.

However, because the volume element  $\Delta x \Delta y \Delta z$  is assumed to be fixed in space, and because the solid grains of a porous medium are essentially incompressible, aquifer deformation and change in porosity can occur only if there is some movement of solid grains across the boundaries of the element, at some finite grain velocity which we designate  $w_g$ . This in turn implies that some pore space, and the interstitial water within that pore space, are also carried across the element boundaries at the velocity  $w_g$  in the deformation process. As noted by Cooper (1966), the Darcy velocity and the associated seepage velocity are actually velocities relative to the grains, or solid matrix, of the porous medium. Thus in a deforming aquifer, the total velocity of the interstitial water relative to a fixed frame of reference is the sum of the seepage velocity and the grain velocity; the total specific discharge, or flow per unit cross-sectional area, is similarly the sum of the Darcy velocity and  $w_g \theta$ , the product of grain velocity and porosity. These total velocity or total specific discharge terms would therefore have to be used in the expression for net solute inflow, e.g., the left-hand sides of equations (1-38)

through (1-40), in order to derive an exact mass balance equation for the deforming system.

In practical problems, the effect of confined storage on solute mass balance is usually very small, and transport equations developed under the rigid-aquifer assumption are an adequate approximation. Where this is not the case, the effect of confined storage can be simulated by including an artificial sink/source term in the governing transport equation, where the source strength is varied to equal the rate of storage accumulation or release associated with aquifer deformation, i.e., the rate of storage accumulation or release in excess of that which would occur in a rigid aquifer.

The most significant storage process observed in the field is unconfined storage, i.e., storage due to movement of the water table or free surface. In terms of the differential equation of groundwater flow, water table storage actually represents a time-varying boundary condition. In practical calculations, however, water table effects are usually treated as an internal storage accumulation or release occurring in the upper part of an aquifer, rather than as a boundary condition. Thus they are represented by the right-hand side of equation (1-22), but using a high value of specific storage, usually taken as the specific yield divided by the thickness of the hydrogeologic interval in which the water table occurs. The solute mass balance in a volume of aquifer which includes the water table cannot be fully represented by equations (1-38) through (1-40), which were derived for a fully saturated volume element in the interior of an aquifer, and contain no term to account for solute gain or loss associated with a rising or falling free surface. In transport simulation, however, the approximating equations at cells or nodes containing a free surface are formulated in terms of the saturated thickness, rather than in terms of a fixed thickness,  $\Delta z$ . The saturated thickness is updated at each time step as the water level changes; thus the volume of water accumulating in or released from storage, and the associated solute mass accumulation or release, can be accounted for in the calculation.

Equations (1-38) through (1-40), in which the partial derivative,  $\partial C/\partial t$ , indicates the rate of change in solute concentration,  $C$ , at a fixed point in space, are called Eulerian expressions (e.g., Daily and Harleman, 1966). Equations of this kind can be used directly in standard numerical solution methods based on the mass-balance approach. Unfortunately, direct solution of the Eulerian form of the advective transport equation is plagued by a serious problem, known as *numerical dispersion*. While we will provide a detailed discussion on this and other topics related to numerical methods for transport simulation in Chapters 5 and 6, we present here an intuitive demonstration of the numerical dispersion phenomenon.

Consider again the apparatus of Figure 1-3, and suppose that initially water having a salt concentration of 10 milligrams per liter (mg/l) circulates



through the system. Suppose that the Darcy velocity in the sand is 10 cm/hr, and the cross-sectional area of the pipe is 100 cm<sup>2</sup>, so that the rate of flow through the sand is 1000 cm<sup>3</sup> per hour, or 1 liter per hour. Assume that the length  $\Delta l$  is 100 cm, and the porosity of the sand is 0.1; thus the pore volume of the element  $A \Delta l$  is 1000 cm<sup>3</sup>, or 1 liter, and the flow rate could be expressed as one pore volume per hour. Finally, assume that the salt concentration of water entering the upstream face is changed abruptly at a time  $t_0$  to 100 mg/l.

Now considering the application of the mass-balance approach over the full volume  $A \Delta l$ . Prior to  $t_0$  salt is transported across the upstream face at a mass rate of 10 milligrams per hour (mg/hr), and is transported out of the volume at the downstream face at the same rate; thus the rate of accumulation of salt mass within the volume is zero. At time  $t_0$  the concentration at the upstream face is changed to 100 mg/l, and the mass rate of salt inflow increases to 100 mg/hr. We apply equation (1-33) to the problem, representing the time derivative,  $\partial C/\partial t$ , as a finite-difference term,  $\Delta C/\Delta t$ , where  $\Delta C$  represents the change in average salt concentration within the volume  $A \Delta l$  over a finite time interval,  $\Delta t$ , which we take as 6 minutes or 0.1 hr; and we assume that the concentration of the water leaving the volume at the outflow face during each time step is equal to the average concentration within the volume at the beginning of the time step. Thus during the first six-minute time step after  $t_0$  we calculate a mass inflow of 100 mg/hr, and a mass outflow of 10 mg/hr. This leads to a rate of mass accumulation in the first time step of 90 mg/hr; at this rate the mass of salt in the volume  $A \Delta l$  increases by 9 mg during the initial time step, causing an increase in concentration of 9 mg/l during that period. In this way we calculate an average concentration of 19 mg/l at the end of the time step. For the second time we again use a mass inflow rate of 100 mg/hr, but we now assume that the outflow concentration is 19 mg/l; thus the mass outflow during the second time step occurs at a rate of 19 mg/hr, and mass accumulation within the volume is calculated as 81 mg/hr. Table 1-1 shows calculated values of average concentration within the volume at the end of each time step using this approach.

In the process of calculation described above we have actually used a finite-difference approach to solve equation (1-33), employing a forward-difference approximation to the time derivative (see Chapter 6). Because we assume that the concentration at the outflow face is equal to the average concentration in volume  $A \Delta l$ , Table 1-1 can be taken as a summary of the calculated outflow concentration as a function of time. If we plot the concentration in Table 1-1 versus time, as shown in Figure 1-5, the result is a smooth curve with the outflow concentration gradually increasing from 10 mg/l and eventually approaching that of the inflow, 100 mg/l.

TABLE 1-1 Calculated Concentration at the Outflow Face for the Mass-Balance Example

Time (hr)	Concentration (mg/l)
0.1	19.0
0.2	27.1
0.3	34.4
0.4	41.0
0.5	46.9
0.6	52.2
0.7	56.9
0.8	61.2
0.9	65.1
1.0	68.6
1.1	71.4
1.2	74.2
1.3	76.8
1.4	79.1
1.5	81.2
1.6	83.1
1.7	84.7
1.8	86.2
1.9	87.5
2.0	88.7

Theoretically, the concentration change at the outflow face for this problem, assuming only advective transport, should show a sharp change from 10 mg/l to 100 mg/l at 1 hour after  $t_0$  (see Figure 1-5). It is clear that the mass-balance method of calculation has introduced a smearing of the concentration-time curve, or "breakthrough" curve, at the outflow face. As we will see in the next chapter, breakthrough curves in nature are never perfectly sharp; there is always a certain amount of spreading, or dispersion, associated with natural velocity variation. The computational effect which we see here mimics this behavior, and hence the term numerical dispersion. It should be pointed out, however, that the numerical dispersion is an artifact of the computation, and is fundamentally unrelated to any physical mechanism.

If instead of using the entire volume  $A \Delta l$  of Figure 1-3 as the basis of our calculation, we were to break that volume into a series of thin slices normal to the pipe, and apply the mass-balance approach in sequence to those slices, we could achieve a better result. Similarly, if we retained the full volume  $A \Delta l$  but happened to use a time step of 1 hour, or in any case a time step closer to the travel time of a fluid particle through the volume of

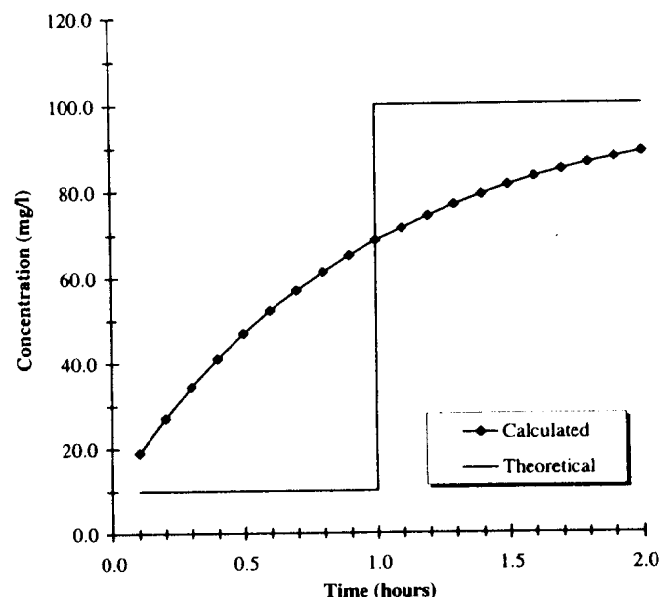


FIGURE 1-5. Outflow concentrations calculated for the purely advective transport example, compared with theoretical outflow concentrations (a constant inflow concentration is assumed).

calculation, we could reduce the numerical dispersion effect. This shows that the numerical dispersion effect is affected by both spatial and temporal discretizations.

### 1.3.2 The Particle Tracking Approach to Advective Transport

Because of the numerical dispersion effect associated with the mass-balance approach, an alternative method based on fluid particle tracking is often used to solve advective transport problems. In this method a concentration value is associated with individual particles of fluid, and the advance of those particles through the region of interest is calculated from an analysis of the flow field. The particle tracking approach is based on the Lagrangian point of view (e.g. Daily and Harleman, 1966; Bear, 1972), in which concentration is associated not with fixed points or volume elements in space, but rather with fluid elements or particles which move with the prevailing flow velocity.

A Lagrangian equation for advective transport can be developed from the mass-balance equation in subscript form, i.e., equation (1-40), if it is kept in mind that  $C$  now refers to the concentration identified with a fluid element or particle which moves with the flow. We may expand the first term on the right side of equation (1-40) using the chain rule as follows:

$$\frac{\partial}{\partial x_i} (v_i C) = v_i \frac{\partial C}{\partial x_i} + C \frac{\partial v_i}{\partial x_i} \quad (1-41)$$

Note that because the subscript notation implies summation over the coordinate directions, the term  $\partial v_i / \partial x_i$  actually represents the flow divergence, or net outflow rate per unit pore volume. In steady-state flow, this term must be equal to the sink/source term  $q_s / \theta$ , which gives the volumetric rate of gain or loss of fluid from sources or sinks, per unit pore volume, i.e.,

$$\frac{\partial v_i}{\partial x_i} = \frac{q_s}{\theta} \quad (1-42)$$

Substituting equations (1-41) and (1-42) into (1-40) and rearranging yields

$$\frac{\partial C}{\partial t} + v_i \frac{\partial C}{\partial x_i} = \frac{q_s}{\theta} (C_s - C) \quad (1-43)$$

The terms on the left side of equation (1-43) define the rate of change of concentration identified with a particle or element of fluid which is moving along a pathline (also referred to as a characteristic curve) of the flow field. The sum of the two terms is referred to as the *substantial derivative* and is designated  $DC/Dt$ , i.e.,

$$\frac{DC}{Dt} = \frac{\partial C}{\partial t} + v_i \frac{\partial C}{\partial x_i} \quad (1-44)$$

Thus equation (1-43) can be written as

$$\frac{DC}{Dt} = \frac{q_s}{\theta} (C_s - C) \quad (1-45)$$

Equation (1-45) can be simplified further by recalling that under the Lagrangian interpretation the concentration,  $C$ , is identified with a moving element or particle; and by noting that in purely advective transport, the concentration carried by particles emerging from a source must be the same

as the concentration associated with the source, and the concentration carried by a particle which enters a sink must be equal to the concentration associated with that particle immediately outside the sink. Thus the terms  $C$  and  $C_s$  of equation (1-45), as interpreted in the Lagrangian context, are equal. Equation (1-45) therefore becomes simply

$$\frac{DC}{Dt} = 0 \quad (1-46)$$

Equation (1-46) is a statement that the concentration identified with a fluid particle does not change with time as the particle traverses a pathline, provided the transport is purely advective. Rather, the particle's concentration at the starting point of the pathline remains its concentration at every point along that pathline. Because particles emanating from a source follow a pathline which originates at the source, they retain the concentration associated with the source along the entire length of the pathline; similarly, particles entering a sink follow a pathline which terminates at the sink, and enter it with the concentration they have carried along the entire pathline. Thus the solution to a problem of purely advective transport using a Lagrangian approach is a matter of defining the pathlines of individual solute particles in the flow regime.

We now return to the problem considered in the previous section, involving the movement of saline water through the apparatus of Figure 1-2; we approach the problem from the Lagrangian point of view, through particle tracking. We begin by placing a number of particles on the planar interface representing the abrupt change in concentration from 10 mg/l to 100 mg/l. We then simply calculate the advance of this planar interface through the sand, beginning at  $t_0$  and moving at a seepage velocity of 100 cm/hr; we interpret the concentration ahead of the interface as 10 mg/l and that behind it as 100 mg/l. Following this method, we calculate the concentration at the outflow face as 10 mg/l until one hour after  $t_0$ , at which time it increases abruptly to 100 mg/l. Note that during the calculation process, no numerical dispersion is introduced, and the results should agree more closely with observation than those obtained using the mass-balance (Eulerian) approach if the transport is predominantly advective.

In the above example there are only two regions, separated by a planar interface which advances uniformly through the sand-packed pipe of Figure 1-2; within each region, concentration has only one value. However, the particle tracking approach has much wider application than this example suggests. For example, in a problem in which the solute distribution is described by a series of three-dimensional surfaces of equal concentration, each of these surfaces may be taken as an interface. The concepts of seepage

velocity and travel time may then be applied to calculate the position of each of these isoconcentration surfaces at successive times, generating a new concentration distribution for each time of calculation. However, even though new concentration distributions are obtained, concentration itself never appears as a variable of calculation under this approach; the calculation involves only the positions, velocities, and times of travel of fluid particles marking the various interfaces.

The effort involved in calculating the advance of an interface depends on the geometry of the interface and the complexity of the flow pattern. In the apparatus of Figure 1-2, an interface would always be a plane at right angles to the pipe; its advance would follow a known direction at a uniform velocity. In a field problem where the flow field is three-dimensional and varying with time, interfaces may advance irregularly and change shape continuously. Calculation of the advance of an interface involves determining the sequence of positions of a large number of particles marking its surface. In the apparatus of Figure 1-2, the velocity is constant in time and the same for all particles. A single calculation of velocity is therefore sufficient, and there is no requirement for bookkeeping to keep track of the positions of a large number of particles at successive times. In the case of a complex three-dimensional interface in the field, the velocities of individual particles on the interface differ from one another and vary through time. Thus the velocity of each particle must be calculated separately, in general using the three-dimensional vector form of Darcy's Law, equations (1-9) through (1-12); and the calculations must be repeated at successive times for all particles. The position of each particle must be updated after each time increment using the velocity, the time increment, and the particle's prior position; and a large amount of computer memory may be needed to store the required information on particle position. However, while the process is more cumbersome, the approach is basically similar to that of calculating the advance of an interface through the pipe of Figure 1-2.

The particle tracking approach and existing computer codes for solving purely advective transport problems are discussed in detail in Chapter 5.