DERIVATION OF EQUATIONS DESCRIBING SOLUTE TRANSPORT IN GROUND WATER

$$+ \frac{E}{V_0} \sum_{j=1}^{S} \frac{\partial m_j}{\partial t} + W^* p^*$$

$$q_j = \frac{-k_{ij}}{\mu} \left(\frac{\partial P}{\partial x_j} + \rho g \frac{\partial z^*}{\partial x_j} \right)$$

$$\frac{\partial}{\partial x_j} \left(T_{ij} \frac{\partial h}{\partial x_j} \right) = S \frac{\partial h}{\partial t} + W$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_j} \left(D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} \left(C V_i \right) - \frac{C' W}{\varepsilon b}$$

$$D_{ij} = \dot{a}_{ijmn} \frac{V_m V_n}{|V|}$$

$$|V| = \sqrt{V_1^2 + V_2^2 + V_3^2}$$

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IN GROUND WATER

By Leonard F. Konikow and David B. Grove

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ABSTRACT

A general equation describing the three-dimensional transport and dispersion of a reacting solute in flowing ground water is derived from the principle of conservation of mass. The derivation presented in this report is more detailed but less rigorous than derivations published previously. The general solute-transport equation relates concentration changes to hydrodynamic dispersion, convective transport, fluid sources and sinks, and chemical reactions. Because both dispersion and convective transport depend on the velocity of ground-water flow, the solute-transport equation must be solved in conjunction with the ground-water flow equation.

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INTRODUCTION

In recent years there has been an increased awareness of problems of ground-water contamination. Reliable predictions of contaminant movement can only be made if we understand and can quantitatively describe the physical and chemical processes that control solute transport in flowing ground water. Several reports have been published recently that develop and present solute-transport equations to compute the concentration of a dissolved chemical species in ground water as a function of space and time. Examples of these reports include Reddell and Sunada (1970), Bear (1972), and Bredehoeft and Pinder (1973). The three main processes affecting solute transport, and consequently chemical concentrations, are convective transport, hydrodynamic dispersion (including diffusion and mechanical dispersion), and chemical reactions. Because convective transport and hydrodynamic dispersion depend on the velocity of ground-water flow, the solute-transport equation must be considered in conjunction with the ground-water flow equation.

Aquifers generally have heterogeneous properties and complex boundary conditions. Therefore, the solution of the partial differential equations that describe the solute-transport processes generally require the use of a deterministic, distributed parameter, digital simulation model. Among the reports that describe or present numerical models to solve the solute-transport equations are Reddell and Sunada (1970), Bredehoeft and Pinder (1973), Pinder (1973), Ahlstrom and Baca (1974), Gupta and others (1975), Grove (1976), and Lantz and others (1976). Furthermore, several documented case histories show that where adequate hydrogeologic data are available, solute-transport models can be used to compute the rates and directions of spreading of contaminants from known or projected sources. Examples of model applications to field problems include Konikow and Bredehoeft (1974), Robertson (1974), Robson (1974), Konikow (1976), and Segol and Pinder (1976).

These models use either finite-difference methods, finite-element methods, or the method of characteristics. The selection of the "best" numerical method depends largely on the nature of the specific field problem, but also depends to some extent on the mathematical background of the analyst. Although solute-transport models are best utilized when the analyst is thoroughly familiar both with the equations and with the numerical algorithm, the increasing availability of documented and published programs affords the opportunity for the use of a model by persons with only minimal familiarity with both.

The basic purpose of this report is to derive a general form of the solute-transport equation from general principles in a more detailed, step-by-step, but less rigorous manner than has been done in previously published literature. The report is intended to serve as an introduction to quantitative modeling of solute-transport processes in ground water. It will also show how the general solute-transport equation can be modified or simplified for application to a variety of different types of field problems. Because of the interrelation between the flow equation and the solute-transport equation, the former will also be presented in some

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detail although not specifically derived. It is assumed that the mathematical background of the reader includes at least a familiarity with partial differential equations.

GROUND-WATER FLOW

General flow equation

A quantitative description of ground-water flow is a prerequisite to accurately representing solute transport in aquifers. A general form of the equation describing the transient flow of a compressible fluid in a nonhomogeneous anisotropic aquifer may be derived by combining Darcy's Law with the continuity equation. By following the developments of Cooper (1966) and of Bredehoeft and Pinder (1973), the general flow equation may be written in cartesian tensor notation as:

$$\frac{\partial}{\partial x_i}\left[\frac{\rho k_{ij}}{\mu}\left(\frac{\partial P}{\partial x_j} + \rho g \frac{\partial z^*}{\partial x_j}\right)\right] = \rho\alpha\frac{\partial P}{\partial t} + \rho_o\epsilon\beta\frac{\partial P}{\partial t}$$

$$+ \frac{\epsilon}{v_o}\sum_{i=1}^{s}\frac{\partial m_i}{\partial t} + W^*\rho^* \tag{1}$$

where k_{ij} is the intrinsic permeability (a second-order tensor), L^2;

ρ is the fluid density, ML^{-3};

μ is the dynamic viscosity, $ML^{-1}T^{-1}$;

P is the fluid pressure, $ML^{-1}T^{-2}$;

g is the gravitational acceleration constant, LT^{-2};

z^* is the elevation of the reference point above a standard datum, L;

W^* $= W^*(x,y,z,t)$ is the volume flux per unit volume (positive sign for outflow and negative for inflow), T^{-1};

ρ^* is the density of the source/sink fluid, ML^{-3};

α is the vertical compressibility coefficient of the medium, $LM^{-1}T^2$;

ρ_o is the fluid density at a reference pressure, temperature, and and concentration, ML^{-3};

ϵ is the effective porosity (dimensionless);

β is the compressibility coefficient of the fluid, $LM^{-1}T^2$;

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v_o is the reference volume of the fluid, L^3;

m_i is the mass of species i in the reference volume v_o, M;

s is the number of species, (dimensionless);

x_i are the cartesian coordinates, L; and

t is time, T.

The summation convention of Cartesian tensor analysis is implied in equation 1. That is, each term is summed over the range of its subscripts. Bredehoeft and Pinder (1973) note that the derivation of equation 1 is based on the following assumptions:

1. The porous medium may only deform vertically.
2. Isothermal conditions prevail.
3. The volume of individual grains remains constant during deformation of the medium.
4. Fluid density is a linear function of pressure and concentration, as indicated by the following relationship:

$$\rho = \rho_o + \rho_o \beta \, (P-P_o) + \frac{1}{v_o} \sum_{i=1}^{s} (m_i - m_{io}) \tag{2}$$

where P_o is the reference fluid pressure, $ML^{-1}T^{-2}$; and

m_{io} is the mass of species i in the reference volume v_o at the reference pressure, M.

5. The permeability is independent of pressure, temperature, and concentration.
6. There is no change in volume caused by mixing fluids of different ionic concentrations.
7. The proportionality constants α and β are independent of pressure and concentration.
8. Hydraulic head gradients are the only significant driving mechanism.
9. The vertical velocity of grains is negligible.

Equations of state

The density and viscosity of ground water are both related to its temperature, pressure, and chemical content. Because isothermal conditions have been assumed, temperature changes need not be considered.

Equation 2 expresses the dependence of density on both the pressure and the mass concentrations of all species. Equation 2 may be rewritten

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in terms of the concentration of a single chemical species of interest as:

$$\rho = \rho_o + \rho_o \beta (P - P_o) + \gamma (C - C_o) \tag{3}$$

where C is the mass concentration per unit volume of solution for the solute species of interest, ML^{-3};

C_o is the concentration of the solute at the reference pressure and temperature, ML^{-3}; and

γ is the constant of proportionality between concentration and fluid density (dimensionless).

If the relationship indicated by equation 3 is substituted for equation 2, then equation 1 may be rewritten as:

$$\frac{\partial}{\partial x_i} \left[\frac{\rho k_{ij}}{\mu} \left(\frac{\partial P}{\partial x_j} + \rho g \frac{\partial z^*}{\partial x_j} \right) \right] = \rho \alpha \frac{\partial P}{\partial t} + \rho_o \epsilon \beta \frac{\partial P}{\partial t}$$

$$+ \epsilon \gamma \frac{\partial C}{\partial t} + W^* \rho^* \tag{4}$$

Viscosity may be similarly expressed as a linear function of concentration by the following:

$$\mu = \mu_o + \lambda (C - C_o) \tag{5}$$

where μ_o is the dynamic viscosity of the fluid at the reference pressure, temperature, and concentration, $ML^{-1}T^{-1}$; and

λ is the constant of proportionality between concentration and viscosity, L^2T^{-1}.

Flow velocity

The seepage velocity, or average interstitial velocity, of ground-water flow may be computed as:

$$V_i = \frac{q_i}{\epsilon} \tag{6}$$

where V_i is the seepage velocity in the direction of x_i, LT^{-1}; and

q_i is the specific discharge, or specific flux, in the direction of x_i, LT^{-1}.

The specific discharge may be computed directly from Darcy's Law, which is written as:

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$$q_i = \frac{-k_{ij}}{\mu} \left(\frac{\partial P}{\partial x_j} + \rho g \frac{\partial z^*}{\partial x_j} \right) \tag{7}$$

Simplifying assumptions

The general flow equation written as equation 4 can be simplified considerably if certain conditions can be satisfied. Several of these are described next.

Homogeneous fluid properties

When changes in concentrations of dissolved chemical species are relatively small, the fluid density and viscosity remain essentially constant. This assumption of homogeneous fluid properties both simplifies the flow equation and allows it to be solved independently from the solute-transport equation. If density is independent of concentration, then the third term on the right side of equation 4 can be eliminated from the flow equation.

We may aim next to express equation 4 in terms of hydraulic head rather than pressure. Following the development of Hubbert (1940), we may define the hydraulic head as:

$$h = z^* + \int_{P_a}^{P} \frac{dP}{\rho g} \tag{8}$$

where h is the hydraulic head, L; and

P_a is atmospheric pressure, $ML^{-1}T^{-2}$.

If we differentiate equation 8 with respect to x_i, for constant density we obtain:

$$\frac{\partial h}{\partial x_i} = \frac{\partial z^*}{\partial x_i} + \frac{1}{\rho g} \frac{\partial P}{\partial x_i} \tag{9}$$

Solving equation 9 for $\frac{\partial P}{\partial x_i}$ yields:

$$\frac{\partial P}{\partial x_i} = \rho g \left(\frac{\partial h}{\partial x_i} - \frac{\partial z^*}{\partial x_i} \right) \tag{10}$$

We may similarly differentiate equation 8 with respect to time to obtain:

$$\frac{\partial h}{\partial t} = \frac{\partial z^*}{\partial t} + \frac{1}{\rho g} \frac{\partial P}{\partial t} \tag{11}$$

Because $\frac{\partial z^*}{\partial t} = 0$, we can express equation 11 as:

$$\frac{\partial P}{\partial t} = \rho g \frac{\partial h}{\partial t} \tag{12}$$

If we next substitute the relations indicated by equations 10 and 12 into equation 4, and then divide both sides of the equation by the constant density, we obtain:

$$\frac{\partial}{\partial x_i} \left(\frac{\rho g}{\mu} k_{ij} \frac{\partial h}{\partial x_j} \right) = g(\rho\alpha + \rho_0 \varepsilon\beta) \frac{\partial h}{\partial t} + W^* \tag{13}$$

Equation 13 may be further reduced if we consider that

$$K_{ij} = \frac{\rho g}{\mu} k_{ij} \tag{14}$$

where K_{ij} is the hydraulic conductivity tensor, LT^{-1}, and that

$$S_s = g(\rho\alpha + \rho_0 \varepsilon\beta) \tag{15}$$

where S_s is the specific storage, L^{-1}.

By substituting equations 14 and 15 into equation 13, we obtain:

$$\frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h}{\partial x_j} \right) = S_s \frac{\partial h}{\partial t} + W^* \tag{16}$$

Two-dimensional areal flow

In many ground-water studies it can be reasonably assumed that ground-water flow is areally two-dimensional. This allows the three-dimensional flow equation to be reduced to the case of two-dimensional areal flow, for which several additional simplifications are possible. The advantages of reducing the dimensionality of the equations include less stringent data requirements, smaller computer storage requirements, and shorter computer execution times to achieve a numerical solution.

An expression similar to equation 16 may be derived for the two-dimensional areal flow of a homogeneous fluid and written as:

$$\frac{\partial}{\partial x_i} \left(K_{ij} b \frac{\partial h}{\partial x_j} \right) = S_s b \frac{\partial h}{\partial t} + W^* b \qquad (17)$$

where b is the saturated thickness of the aquifer, L, and it is assumed that the hydraulic conductivity, specific storage, and hydraulic head represent vertically integrated mean values (Cooley, 1974).

The transmissivity of the aquifer may be defined as:

$$T_{ij} = K_{ij} b \qquad (18)$$

where T_{ij} is the transmissivity, $L^2 T^{-1}$.

Similarly, the storage coefficient of the aquifer may be defined as:

$$S = S_s b \qquad (19)$$

where S is the storage coefficient (dimensionless).

After substituting the relationships indicated by equations 18 and 19 into equation 17, we obtain:

$$\frac{\partial}{\partial x_i} \left(T_{ij} \frac{\partial h}{\partial x_j} \right) = S \frac{\partial h}{\partial t} + W \qquad (20)$$

where $W = W(x,y,t) = W^* b$ is the volume flux per unit area, LT^{-1}.

Although fluid sources and sinks may vary in space and time, they have been lumped into one term (W) in the previous development. There are several possible ways to compute W. If we consider only sources and sinks such as (1) direct withdrawal or recharge, such as pumpage from a well, well injection, or evapotranspiration, and (2) steady-state leakage into or out of the aquifer through a confining layer, streambed, or lake bed, then for the case of two-dimensional horizontal flow, the source/sink terms may be specifically expressed as:

$$W(x,y,t) = Q(x,y,t) - \frac{K_z}{m} (H_s - h) \qquad (21)$$

where Q is the rate of withdrawal (positive sign) or recharge (negative sign), LT^{-1};

K_z is the vertical hydraulic conductivity of the confining layer, streambed, or lake bed, LT^{-1};

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m is the thickness of the confining layer, streambed, or lake bed, L; and

H_s is the hydraulic head in the source bed, stream, or lake, L.

Alignment of coordinate axes

The cross-product terms of the permeability tensor drop out when the coordinate axes are aligned with the principal axes of the tensor (Bredehoeft, 1969); that is, $k_{ij} = 0$ when $i \neq j$. Therefore, the only permeability terms with possible nonzero values are k_{xx}, k_{yy}, and k_{zz}. This assumption simplifies the general flow equation, which can now be rewritten to include all permeability terms as:

$$\frac{\partial}{\partial x}\left[\frac{\rho k_{xx}}{\mu}\left(\frac{\partial P}{\partial x} + \rho g \frac{\partial z^*}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[\frac{\rho k_{yy}}{\mu}\left(\frac{\partial P}{\partial y} + \rho g \frac{\partial z^*}{\partial y}\right)\right]$$

$$+ \frac{\partial}{\partial z}\left[\frac{\rho k_{zz}}{\mu}\left(\frac{\partial P}{\partial z} + \rho g \frac{\partial z^*}{\partial z}\right)\right] = \rho\alpha \frac{\partial P}{\partial t} + \rho_o \varepsilon\beta \frac{\partial P}{\partial t} + \varepsilon\gamma \frac{\partial C}{\partial t} + W^*\rho^* \qquad (22)$$

Darcy's Law may be written similarly for the three flow directions as:

$$q_x = -\frac{k_{xx}}{\mu}\left(\frac{\partial P}{\partial x} + \rho g \frac{\partial z^*}{\partial x}\right) \qquad (23a)$$

$$q_y = -\frac{k_{yy}}{\mu}\left(\frac{\partial P}{\partial y} + \rho g \frac{\partial z^*}{\partial y}\right) \qquad (23b)$$

$$q_z = -\frac{k_{zz}}{\mu}\left(\frac{\partial P}{\partial z} + \rho g \frac{\partial z^*}{\partial z}\right) \qquad (23c)$$

For the case of two-dimensional areal flow, if the coordinate axes are aligned with the principal directions of the transmissivity tensor, equation 20 may be written as:

$$\frac{\partial}{\partial x}\left(T_{xx} \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy} \frac{\partial h}{\partial y}\right) = S \frac{\partial h}{\partial t} + W \qquad (24)$$

SOLUTE-TRANSPORT EQUATION

Derivation of general transport equation

An equation describing the three-dimensional transport and dispersion of a reacting dissolved chemical in flowing ground water will be derived from the principle of conservation of mass (continuity condition). The derivation presented here is based on the developments of Reddell and Sunada (1970), Bear (1972), and Bredehoeft and Pinder (1973).

The principle of conservation of mass requires that the net mass of solute entering or leaving a specified volume of aquifer during a given time interval must equal the accumulation or loss of mass stored in that volume during the interval. This may be expressed in a verbal equation as:

(Rate of Solute Accumulation)

= (Rate of Solute Inflow) − (Rate of Solute Outflow)

+ (Rate of Chemical Production by Reactions)   (25)

This relationship may then be expressed mathematically by considering all fluxes into and out of a representative elementary volume (REV), as described by Bear (1972, p. 19). The REV shown in figure 1 is centered at coordinates (x, y, z) and has dimensions (Δx, Δy, Δz).

First we will determine fluxes in the x-direction. We know that at the center of the REV the mass flux of solute in the x-direction across the y-z plane (face IJKL) is equal to $(CV_x^* \, \varepsilon \Delta y \Delta z)$, where C is the concentration of the solute (ML^{-3}), V_x^* is the instantaneous mass velocity of the solute (LT^{-1}), and Δy and Δz are the dimensions (L) of face IJKL. Note that the term $(\varepsilon \Delta y \Delta z)$ simply represents the total effective cross-sectional area through which flow is occurring.

We need expressions for the fluxes across the outer faces ABCD and EFGH. The difference between the mass flux of solute across face ABCD and face IJKL equals the rate of change of mass flux in the x-direction times the distance between these two faces. The rate of change of the mass flux of solute in the x-direction equals $\frac{\partial}{\partial x}(CV_x^* \, \varepsilon \Delta y \Delta z)$, and the distance from the center to face ABCD is (−Δx/2). Thus, the mass flux through face ABCD equals

$$CV_x^* \, \varepsilon \Delta y \Delta z - \frac{\partial}{\partial x}(CV_x^* \, \varepsilon \Delta y \Delta z)\frac{\Delta x}{2}$$

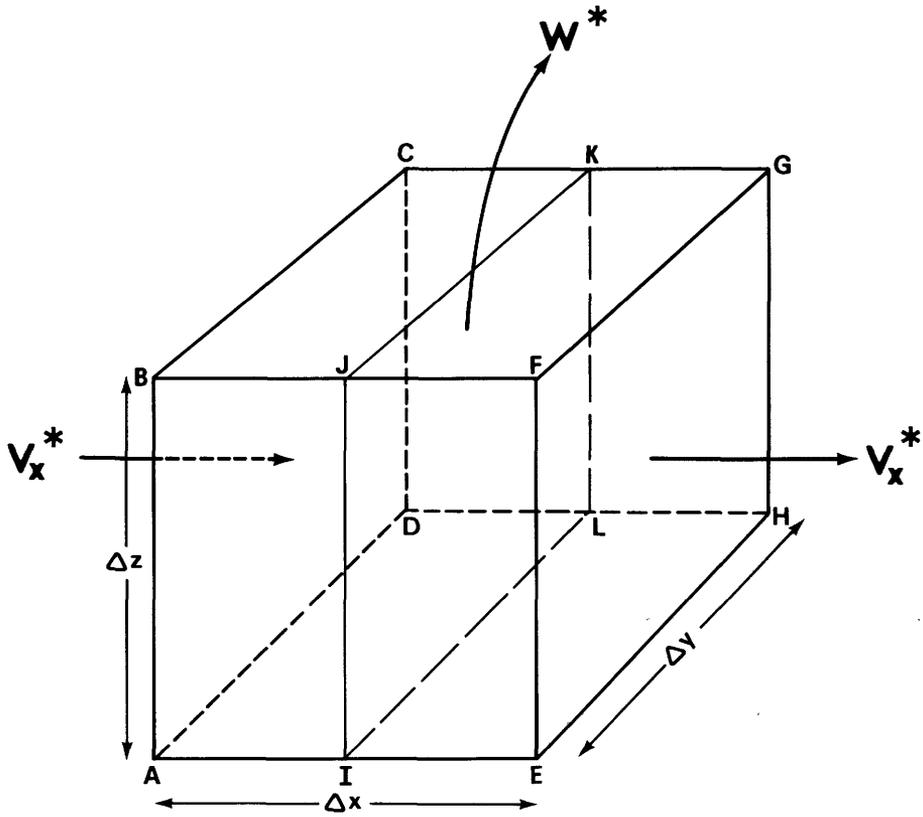Similarly, the distance from the center to face EFGH is (+Δx/2) and the mass flux through face EFGH is given by

Figure 1.--Representative elementary volume (REV) of aquifer.

$$CV_x{}^* \ \varepsilon \Delta y \Delta z + \frac{\partial}{\partial x} \ (CV_x{}^* \ \varepsilon \Delta y \Delta z)\frac{\Delta x}{2}$$

The net mass flux of the solute entering or leaving the REV in the x-direction equals the difference (input-output) between the two previous terms:

$$(\text{Net Mass Flux})_x = \left[CV_x{}^* \ \varepsilon \Delta y \Delta z - \frac{\partial}{\partial x} \ (CV_x{}^* \ \varepsilon \Delta y \Delta z)\frac{\Delta x}{2} \right]$$

$$- \left[CV_x{}^* \ \varepsilon \Delta y \Delta z + \frac{\partial}{\partial x} \ (CV_x{}^* \ \varepsilon \Delta y \Delta z)\frac{\Delta x}{2} \right]$$

$$= - \frac{\partial}{\partial x} \ (CV_x{}^* \ \varepsilon \Delta y \Delta z)\Delta x \tag{26}$$

This equation can also be derived by writing a Taylor series for the mass flux term about the point (x, y, z) (Reddell and Sunada, 1970, p. 39). Note that if the value of the derivative in the x-direction (equation 26) is negative, then the mass flux of solute entering through face ABCD is greater than the mass leaving through face EFGH. If all other fluxes balance, there will then be a positive accumulation of solute mass in the REV. Conversely, if the derivative is positive, there will be a decrease over time of solute mass stored in the REV.

It can similarly be shown that for the y-direction:

$$(\text{Net Mass Flux})_y = - \frac{\partial}{\partial y} \ (CV_y{}^* \ \varepsilon \Delta x \Delta z)\Delta y \tag{27a}$$

and for the z-direction:

$$(\text{Net Mass Flux})_z = - \frac{\partial}{\partial z} \ (CV_z{}^* \ \varepsilon \Delta x \Delta y)\Delta z \tag{27b}$$

Solute may also enter or leave the REV as a flux through a source or sink (W). This may be expressed mathematically as:

$$(\text{Source/Sink Mass Flux})_{REV} = C'W^*\Delta x \Delta y \Delta z \tag{28}$$

where C' is the concentration of the solute in the source or sink fluid, ML^{-3}.

If a sink (withdrawal) is considered positive in sign and a source (recharge or injection) is considered negative in sign, then when all other fluxes balance, a positive W must be balanced by a decrease over time of solute mass stored in the REV (negative $\frac{\partial C}{\partial t}$), and vice versa. Note that for a sink C' is equivalent to the concentration in the aquifer at the location of the sink.

A particular solute may also be added to or removed from solution within the REV by the effects of chemical reactions. Examples of such reactions include radioactive decay, ion exchange, and adsorption. The amount of solute that is produced (that is, added to or removed from solution) within the REV is equal to the rate of production of the solute times the volume of solution and may be expressed as:

$$\text{(Solute Mass Produced)}_{REV} = \epsilon \Delta x \Delta y \Delta z \sum_{k=1}^{s} R_k \qquad (29)$$

where R_k is the rate of production of the solute in reaction k of s different reactions (positive for addition of solute and negative for removal), $ML^{-3}T^{-1}$.

The conservation of mass for a given solute may be expressed in a continuity equation by combining the terms in equations 26, 27a, 27b, 28, and 29, resulting in:

$$\frac{\partial}{\partial t} (C\epsilon \Delta x \Delta y \Delta z) = - \frac{\partial}{\partial x} (CV_x{}^* \epsilon \Delta y \Delta z) \Delta x$$

$$- \frac{\partial}{\partial y} (CV_y{}^* \epsilon \Delta x \Delta z) \Delta y - \frac{\partial}{\partial z} (CV_z{}^* \epsilon \Delta x \Delta y) \Delta z$$

$$- C'W^* \Delta x \Delta y \Delta z + \epsilon \Delta x \Delta y \Delta z \sum_{k=1}^{s} R_k \qquad (30)$$

If we assume that changes over time in porosity of the aquifer are not significant and Δx, Δy, and Δz are constants, then their derivatives equal zero. Using an indicial notation to represent directions in which x_1, x_2, and x_3 correspond to the x-, y-, and z-directions respectively, equation 30 can be rewritten as:

$$\epsilon \Delta x_1 \Delta x_2 \Delta x_3 \frac{\partial C}{\partial t} = - \Delta x_1 \Delta x_2 \Delta x_3 \frac{\partial}{\partial x_i} (CV_i{}^* \epsilon) - C'W^* \Delta x_1 \Delta x_2 \Delta x_3$$

$$+ \epsilon \Delta x_1 \Delta x_2 \Delta x_3 \sum_{k=1}^{s} R_k \qquad (31)$$

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Dividing both sides of equation 31 by $(\Delta x_1 \Delta x_2 \Delta x_3)$ to remove the common factors results in:

$$\varepsilon \frac{\partial C}{\partial t} = - \frac{\partial}{\partial x_i} (CV_i{}^* \varepsilon) - C'W^* + \varepsilon \sum_{k=1}^{s} R_k \qquad (32)$$

The instantaneous mass flux of the solute is given as $CV_i{}^*$. As shown by Bear (1972, p. 101), this flux can be separated into two parts:

$$CV_i{}^* = CV_i + C\overset{\circ}{V}_i \qquad (33)$$

where $\overset{\circ}{V}_i$ is the deviation of the mass average velocity of the solute from the average insterstitial velocity of the fluid $(\overset{\circ}{V}_i = V_i{}^* - V_i)$, LT^{-1}.

The term CV_i represents the convective flux of solute carried by the average fluid motion through the REV. Neglecting diffusion, the term $C\overset{\circ}{V}_i$ represents the dispersive flux resulting from velocity fluctuations.

Bear (1972, p. 101) also shows that the dispersive flux can be approximated by:

$$C\overset{\circ}{V}_i = - D_{ij} \frac{\partial C}{\partial x_j} \qquad (34)$$

where D_{ij} is the coefficient of mechanical dispersion (a second-order tensor), $L^2 T^{-1}$.

Equation 34 indicates that the dispersive flux is directly proportional to the concentration gradient and occurs in a direction from higher concentrations towards lower concentrations. The form of equation 34 is analogous to Fick's Law describing diffusive flux, as described by Bear (1972, p. 78). In considering flowing ground water, diffusive fluxes are assumed to be negligible in comparison to dispersive fluxes. If diffusion is negligible, the coefficient of mechanical dispersion is equivalent to the coefficient of hydrodynamic dispersion described by Bear (1972, p. 606).

Coupling between forces of one type and fluxes of another type are discussed by Bear (1972, p. 85-90). By following the development of Bredehoeft and Pinder (1973), and by assuming that the only significant driving mechanism is the gradient of hydraulic head and that Darcy's Law is fully valid, we eliminate the necessity of considering coupled processes.

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As a result of substituting equation 34 into equation 33, the instantaneous mass flux may be expressed in terms of the dispersion coefficient as:

$$CV_i^* = CV_i - D_{ij} \frac{\partial C}{\partial x_j} \tag{35}$$

Equation 35 can next be substituted into equation 32 to yield:

$$\varepsilon \frac{\partial C}{\partial t} = - \frac{\partial}{\partial x_i} \left[\varepsilon \left(CV_i - D_{ij} \frac{\partial C}{\partial x_j} \right) \right] - C'W^* + \varepsilon \sum_{k=1}^{s} R_k \tag{36}$$

which is equivalent to:

$$\varepsilon \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left(\varepsilon D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (\varepsilon CV_i)$$

$$- C'W^* + \varepsilon \sum_{k=1}^{s} R_k \tag{37}$$

If spatial changes in porosity are negligible, both sides of equation 37 can be divided by ε to produce:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (CV_i) - \frac{C'W^*}{\varepsilon} + \sum_{k=1}^{s} R_k \tag{38}$$

which is a general equation for computing the concentration of a single dissolved chemical species in flowing ground water.

For the general case of three-dimensional transport of a single dissolved chemical species in flowing ground water, equations 4 and 38 must be solved simultaneously. This requires the use of the auxiliary equations 3, 5, 6, and 7.

At this point it is of value to consider in more detail the second term on the right side of equation 38, which describes convective transport. This term may be expanded as follows:

$$- \frac{\partial}{\partial x_i} (CV_i) = - C \frac{\partial V_i}{\partial x_i} - V_i \frac{\partial C}{\partial x_i} \tag{39}$$

It is often assumed in cases of steady-state flow that the divergence of velocity ($\partial V_i / \partial x_i$) equals zero and the first term on the right side of equation 39 can be eliminated. However, as shown by the following

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development, this would be an erroneous assumption if any fluid sources are present or if fluid density varies in space.

By using the definition of V_i indicated by equation 6, we may rewrite the first term on the right side of equation 39 as:

$$-C \frac{\partial V_i}{\partial x_i} = - \frac{C}{\varepsilon} \frac{\partial q_i}{\partial x_i} \qquad (40)$$

Next, substitution of the definition of q_i from equation 7 into equation 40 gives:

$$-C \frac{\partial V_i}{\partial x_i} = - \frac{C}{\varepsilon} \frac{\partial}{\partial x_i} \left[\frac{-k_{ij}}{\mu} \left(\frac{\partial P}{\partial x_j} + \rho g \frac{\partial z^*}{\partial x_j} \right) \right] \qquad (41)$$

If we multiply the expression within the brackets by ρ/ρ and substitute the relationships shown in equations 4 and 7, we obtain:

$$-C \frac{\partial V_i}{\partial x_i} = \frac{C\alpha}{\varepsilon} \frac{\partial P}{\partial t} + \frac{C\rho_o \beta}{\rho} \frac{\partial P}{\partial t} + \frac{C\gamma}{\rho} \frac{\partial C}{\partial t} + \frac{CW^* \rho^*}{\varepsilon\rho} + \rho q_i \frac{\partial (1/\rho)}{\partial x_i} \qquad (42)$$

If steady-state flow existed, $\frac{\partial P}{\partial t} = 0$ and the first two terms on the right side are eliminated. Although the third term may be insignificant, the fourth term, which describes sources and sinks, would have to be included in the analysis, as would the fifth term, which is related to the spatial variability of fluid density.

Two-dimensional areal solute transport

A solute-transport equation for problems involving two-dimensional areal flow may be derived in a manner analogous to the previous derivation of a general three-dimensional equation by assuming that vertical variations in head and concentration are negligible. Consider the total volume of aquifer under a representative square area, as shown in figure 2. Note that the vertical dimension is represented by the saturated thickness, b, and that b may vary within the representative area. In this case the mass flux through face ABCD is approximately equal to

$$CV_x^* \, \varepsilon \Delta y b - \frac{\partial}{\partial x} \left(CV_x^* \, \varepsilon \Delta y b \right) \frac{\Delta x}{2}$$
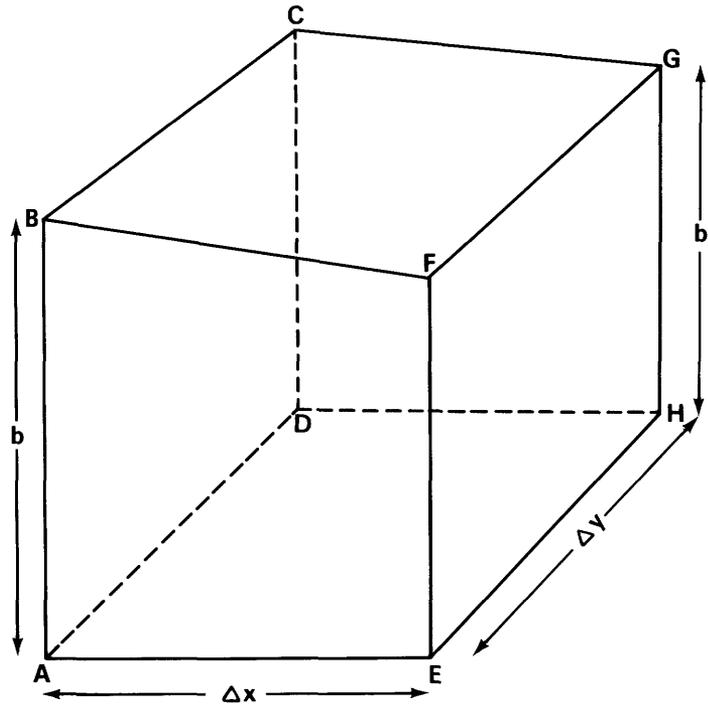
Figure 2.--Representative volume of aquifer having variable saturated thickness.

Similarly, the mass flux through face EFGH may be given by

$$CV_x^* \, \varepsilon \Delta yb + \frac{\partial}{\partial x}\left(CV_x^* \, \varepsilon \Delta yb\right)\frac{\Delta x}{2}$$

The net mass flux of the solute entering or leaving the representative volume thus equals the difference between the two previous terms:

$$(\text{Net Mass Flux})_x = -\frac{\partial}{\partial x}\left(CV_x^* \, \varepsilon \Delta yb\right)\Delta x \tag{43}$$

It can also be shown in the same manner that for the y-direction:

$$(\text{Net Mass Flux})_y = -\frac{\partial}{\partial y}\left(CV_y^* \, \varepsilon \Delta xb\right)\Delta y \tag{44}$$

In the case of two-dimensional areal flow, it is assumed that any flux across the upper or lower faces of the representative volume is included in the source/sink term. Solute entering or leaving the representative volume through a source or sink may be expressed mathematically as:

$$(\text{Source/Sink Mass Flux}) = C'W\Delta x\Delta y \tag{45}$$

Solute added to or removed from solution within the representative volume by the effects of chemical reactions may be expressed as:

$$(\text{Solute Mass Produced}) = \varepsilon \Delta x \Delta yb \sum_{k=1}^{s} R_k \tag{46}$$

The conservation of mass for a given solute may be expressed in a continuity equation by combining the terms in equations 43, 44, 45, and 46, resulting in:

$$\frac{\partial}{\partial t}\left(C\varepsilon\Delta x\Delta yb\right) = -\frac{\partial}{\partial x}\left(CV_x^* \, \varepsilon \Delta yb\right)\Delta x$$

$$-\frac{\partial}{\partial y}\left(CV_y^* \, \varepsilon \Delta xb\right)\Delta y$$

$$- C'W\Delta x\Delta y + \varepsilon \Delta x \Delta yb \sum_{k=1}^{s} R_k \tag{47}$$

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If ε, Δx, and Δy are constants, equation 47 may be rewritten as:

$$\varepsilon \Delta x \Delta y \frac{\partial (Cb)}{\partial t} = - \varepsilon \Delta x \Delta y \frac{\partial}{\partial x} \left(CV_x^* \, b \right)$$

$$- \varepsilon \Delta x \Delta y \frac{\partial}{\partial y} \left(CV_y^* \, b \right)$$

$$- C'W\Delta x \Delta y + \varepsilon \Delta x \Delta y b \sum_{k=1}^{s} R_k \qquad (48)$$

Dividing both sides of equation 48 by ($\varepsilon \Delta x \Delta y$) results in:

$$\frac{\partial (Cb)}{\partial t} = - \frac{\partial}{\partial x} \left(CV_x^* \, b \right) - \frac{\partial}{\partial y} \left(CV_y^* \, b \right)$$

$$- \frac{C'W}{\varepsilon} + b \sum_{k=1}^{s} R_k \qquad (49)$$

By expressing equation 49 in tensor notation and substituting equation 35, written for two dimensions, into equation 49, we obtain:

$$\frac{\partial (Cb)}{\partial t} = - \frac{\partial}{\partial x_i} \left[b \left(CV_i - D_{ij} \frac{\partial C}{\partial x_j} \right) \right]$$

$$- \frac{C'W}{\varepsilon} + b \sum_{k=1}^{s} R_k \qquad (50)$$

which is equivalent to:

$$\frac{\partial (Cb)}{\partial t} = \frac{\partial}{\partial x_i} \left(bD_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} \left(bCV_i \right)$$

$$- \frac{C'W}{\varepsilon} + b \sum_{k=1}^{s} R_k \qquad (51)$$

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The left side of equation 49 may be expanded as:

$$\frac{\partial(Cb)}{\partial t} = C \frac{\partial b}{\partial t} + b \frac{\partial C}{\partial t} \tag{52}$$

Substituting equation 52 into equation 51 and solving for $\partial C/\partial t$ results in:

$$\frac{\partial C}{\partial t} = \frac{1}{b} \frac{\partial}{\partial x_i} \left(bD_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{1}{b} \frac{\partial}{\partial x_i} \left(bCV_i \right)$$

$$- \frac{C}{b} \frac{\partial b}{\partial t} - \frac{C'W}{\varepsilon b} + \sum_{k=1}^{s} R_k \tag{53}$$

If the saturated thickness is constant in space, the spatial derivatives of b are equal to zero. Under these conditions, equation 53 can be further simplified to:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} \left(CV_i \right)$$

$$- \frac{C'W}{\varepsilon b} - \frac{C}{b} \frac{\partial b}{\partial t} + \sum_{k=1}^{s} R_k \tag{54}$$

The two-dimensional solute-transport equation can be reduced further if changes in saturated thickness over time are negligible and if the solute is not affected by chemical reactions. Under these conditions equation 54 may be simplified to:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} \left(CV_i \right) - \frac{C'W}{\varepsilon b} \tag{55}$$

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The difference between equation 53 and equation 54 can be presented more explicitly by expanding the first two terms on the right side of equation 53. After combining terms, equation 53 may then be rewritten as:

$$\frac{\partial C}{\partial t} = \frac{1}{b}\left[D_{ij}\frac{\partial C}{\partial x_j} - CV_i\right]\frac{\partial b}{\partial x_i} + \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right)$$

$$-\frac{\partial(CV_i)}{\partial x_i} - \frac{C'W}{\varepsilon b} - \frac{C}{b}\frac{\partial b}{\partial t} + \sum_{k=1}^{s}R_k \qquad (56)$$

Thus, the difference between equations 53 and 54 is equal to:

$$\frac{1}{b}\left[D_{ij}\frac{\partial C}{\partial x_j} - CV_i\right]\frac{\partial b}{\partial x_i}$$

In other words, the error in computed concentrations caused by assuming that the saturated thickness is uniform, when it actually varies in space, is inversely proportional to the saturated thickness and directly proportional to the divergence of the saturated thickness. If the rate of change in saturated thickness is small compared to the total saturated thickness, the simpler equation 54 can be used as a reasonable approximation to equation 53.

We may also rewrite equation 53 by expanding the convective transport term, as was done by equation 39 to obtain:

$$\frac{\partial C}{\partial t} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - V_i\frac{\partial C}{\partial x_i} - \frac{C}{b}\frac{\partial(V_i b)}{\partial x_i}$$

$$-\frac{C}{b}\frac{\partial b}{\partial t} - \frac{C'W}{\varepsilon b} + \sum_{k=1}^{s}R_k \qquad (57)$$

The third, fourth, and fifth terms on the right side of equation 57 may be combined into one term as follows:

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$$-\frac{C}{b}\frac{\partial(V_i b)}{\partial x_i} - \frac{C}{b}\frac{\partial b}{\partial t} - \frac{C'W}{\varepsilon b}$$

$$= \frac{C\left[-\dfrac{\partial(\varepsilon V_i b)}{\partial x_i} - \varepsilon\dfrac{\partial b}{\partial t}\right] - C'W}{\varepsilon b} \tag{58}$$

It can be shown from equations 6, 7, 9, 14, and 18 that:

$$\varepsilon V_i b = - T_{ij}\frac{\partial h}{\partial x_j} \tag{59}$$

Thus, from equation 20 we can state that:

$$-\frac{\partial}{\partial x_i}\left(\varepsilon V_i b\right) = S\frac{\partial h}{\partial t} + W \tag{60}$$

By substituting equation 60 into equation 58 we can rewrite equation 57 as:

$$\frac{\partial C}{\partial t} = \frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - V_i\frac{\partial C}{\partial x_i}$$

$$+ \frac{C\left[S\dfrac{\partial h}{\partial t} + W - \varepsilon\dfrac{\partial b}{\partial t}\right] - C'W}{\varepsilon b}$$

$$+ \sum_{k=1}^{s} R_k \tag{61}$$

For the case of a water-table aquifer we may assume:

$$S = S_y \tag{62}$$

where S_y is the specific yield of the aquifer (dimensionless). We may also assume that in the case of a water-table aquifer, the Dupuit-Forchheimer assumptions hold (Bear, 1972, p. 361-366), so that:

$$\frac{\partial b}{\partial t} = \frac{\partial h}{\partial t} \tag{63}$$

For the case of an artesian aquifer we can normally assume that:

$$\frac{\partial b}{\partial t} = 0 \tag{64}$$

If changes in saturated thickness over time and space are both negligible, equation 49 may be simplified to:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - V_i\frac{\partial C}{\partial x_i}$$

$$+ \frac{C\left(S\frac{\partial h}{\partial t} + W\right) - C'W}{\varepsilon b} + \sum_{k=1}^{s} R_k \tag{65}$$

In the case of steady-state flow, the third term on the right side of equation 65 may be simplified to:

$$\frac{C\left(S\frac{\partial h}{\partial t} + W\right) - C'W}{\varepsilon b} = \frac{W(C-C')}{\varepsilon b} \tag{66}$$

It is interesting to note that when W represents withdrawal only, then C' = C and the right side of equation 66 becomes equal to zero. Therefore, withdrawals from the aquifer produce concentration changes only indirectly through the effects of the withdrawals on the velocity field, rather than by any direct effect on the mass or concentration of solutes.

If vertical variations of head or concentration are significant, then the two-dimensional equations previously derived would not precisely describe areal solute transport. Cooley (written commun., 1976) shows that when a two-dimensional solute-transport equation is derived with a more rigorous vertical integration of the three-dimensional equation, the third dimension is not actually eliminated in converting to areal coordinates but instead is transformed to boundary conditions.

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Dispersion coefficient

The solution of the solute-transport equation requires consideration of the dispersion coefficient. Because of its tensorial properties, its consideration may not appear to be straightforward. Hence, we will next consider this coefficient in more detail.

Bear (1972, p. 580-581) states that hydrodynamic dispersion is the macroscopic outcome of the actual movements of individual tracer particles through the pores and that it includes two processes. One process is mechanical dispersion, which depends upon both the flow of the fluid and the nature of the pore system through which the flow takes place. The second process is molecular and ionic diffusion, which because it depends on time, is more significant at low flow velocities. Bear (1972) further states that the separation between the two processes is artificial. In developing our model we assume for flowing ground-water systems that the definable contribution of molecular and ionic diffusion to hydrodynamic dispersion is negligible.

The relationship between the dispersion coefficient, the fluid flow, and the nature of the pore system is given in tensor notation by Scheidegger (1961, p. 3275) as:

$$D_{ij} = a_{ijmn} \frac{V_m V_n}{|V|} \tag{67}$$

where a_{ijmn} is the dispersivity of the porous medium (a fourth-order tensor), L;

V_m and V_n are the components of the flow velocity of the fluid in the m and n directions, respectively, LT^{-1}; and

$|V|$ is the magnitude of the velocity vector, LT^{-1}.

Scheidegger (1961, p. 3275) states that the dispersivity tensor possesses 81 components, but that even in the case of an anisotropic medium, symmetry properties reduce the number of components to 36. Both Scheidegger (1961) and Bear (1972) show that the dispersivity of an isotropic porous medium can be defined by two constants. These are the longitudinal dispersivity of the medium, a_L, and the transverse dispersivity of the medium a_T. For an isotropic porous medium the components of the dispersivity tensor in three dimensions ($i,j = 1,2,3$) are:

$$a_{iiii} = a_L \tag{68a}$$

$$a_{iijj} = a_T \tag{68b}$$

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$$a_{iiij} = a_{iiji} = a_{ijii} = a_{ijjj} = 0 \tag{68c}$$

$$a_{ijij} = a_{ijji} = \frac{1}{2}(a_L - a_T) \tag{68d}$$

The components of the dispersion coefficient for three-dimensional flow may be stated explicitly by expanding equation 67 for a range of three on i and j. After eliminating terms with coefficients that equal zero (shown by equation 68c), we obtain:

$$D_{11} = a_{1111}\frac{v_1 v_1}{|v|} + a_{1122}\frac{v_2 v_2}{|v|} + a_{1133}\frac{v_3 v_3}{|v|} \tag{69a}$$

$$D_{22} = a_{2211}\frac{v_1 v_1}{|v|} + a_{2222}\frac{v_2 v_2}{|v|} + a_{2233}\frac{v_3 v_3}{|v|} \tag{69b}$$

$$D_{33} = a_{3311}\frac{v_1 v_1}{|v|} + a_{3322}\frac{v_2 v_2}{|v|} + a_{3333}\frac{v_3 v_3}{|v|} \tag{69c}$$

$$D_{12} = D_{21} = a_{1212}\frac{v_1 v_2}{|v|} + a_{1221}\frac{v_2 v_1}{|v|} \tag{69d}$$

$$D_{13} = D_{31} = a_{1313}\frac{v_1 v_3}{|v|} + a_{1331}\frac{v_3 v_1}{|v|} \tag{69e}$$

$$D_{23} = D_{32} = a_{2323}\frac{v_2 v_3}{|v|} + a_{2332}\frac{v_3 v_2}{|v|} \tag{69f}$$

If we substitute the identities presented in equations 68a and b into equations 69a, b, and c, we obtain directly:

$$D_{11} = a_L\frac{v_1 v_1}{|v|} + a_T\frac{v_2 v_2}{|v|} + a_T\frac{v_3 v_3}{|v|} \tag{70a}$$

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$$D_{22} = a_T \frac{V_1 V_1}{|v|} + a_T \frac{V_2 V_2}{|v|} + a_T \frac{V_3 V_3}{|v|} \qquad (70b)$$

$$D_{33} = a_T \frac{V_1 V_1}{|v|} + a_T \frac{V_2 V_2}{|v|} + a_L \frac{V_3 V_3}{|v|} \qquad (70c)$$

Next, by substituting the identities given by equation 68d into equations 69d, e, and f, we see that:

$$D_{12} = D_{21} = (a_L - a_T) \frac{V_1 V_2}{|v|} \qquad (71a)$$

$$D_{13} = D_{31} = (a_L - a_T) \frac{V_1 V_3}{|v|} \qquad (71b)$$

$$D_{23} = D_{32} = (a_L - a_T) \frac{V_2 V_3}{|v|} \qquad (71c)$$

Scheidegger (1961) and Bachmat and Bear (1964) also show that for a Cartesian coordinate system x_i in which one of the axes, say x_1, coincides with the direction of the average velocity, then $V_1 = |V|$ and $V_2 = 0$. Substituting these relations into equations 70 and 71 we obtain:

$$D_{11} = a_L |V| = D_L \qquad (72a)$$

$$D_{22} = D_{33} = a_T |V| = D_T \qquad (72b)$$

$$D_{12} = D_{21} = D_{13} = D_{31} = D_{23} = D_{32} = 0 \qquad (72c)$$

where D_L and D_T are respectively the longitudinal and transverse dispersion coefficients, $L^2 T^{-1}$

Solving equations 72a and b for a_L and a_T results in:

$$a_L = \frac{D_L}{|v|} \tag{73a}$$

$$a_T = \frac{D_T}{|v|} \tag{73b}$$

Introducing equations 73a and b into equations 70 and 71 produces:

$$D_{11} = D_L \frac{(V_1)^2}{|v|^2} + D_T \frac{(V_2)^2}{|v|^2} + D_T \frac{(V_3)^2}{|v|^2} \tag{74a}$$

$$D_{22} = D_T \frac{(V_1)^2}{|v|^2} + D_L \frac{(V_2)^2}{|v|^2} + D_T \frac{(V_3)^2}{|v|^2} \tag{74b}$$

$$D_{33} = D_T \frac{(V_1)^2}{|v|^2} + D_T \frac{(V_2)^2}{|v|^2} + D_L \frac{(V_3)^2}{|v|^2} \tag{74c}$$

$$D_{12} = D_{21} = (D_L - D_T) \frac{V_1 V_2}{|v|^2} \tag{74d}$$

$$D_{13} = D_{31} = (D_L - D_T) \frac{V_1 V_3}{|v|^2} \tag{74e}$$

$$D_{23} = D_{32} = (D_L - D_T) \frac{V_2 V_3}{|v|^2} \tag{74f}$$

Equation 74 defines the local transformation of D_{ij} from orthogonal axes, in which x_1 is parallel to V_1, to global cartesian axes. Note that while D_{11}, D_{22}, and D_{33} must have positive values, it is possible for the cross-product terms (equations 74d, e, and f) to have negative values.

For the case of two-dimensional flow, all components and terms in equation 74 that have a subscript 3 are eliminated.

The magnitude of the velocity, $|V|$, is defined as:

$$|V| = \sqrt{V_1^2 + V_2^2 + V_3^2} \tag{75}$$

In summary, the components of the dispersion tensor that must be evaluated for three-dimensional flow in an isotropic porous medium are:

$$D_{ij} = \begin{vmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{vmatrix} = \begin{vmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{vmatrix} \tag{76}$$

SUMMARY

A general equation describing the three-dimensional transport and dispersion of a reacting dissolved chemical in flowing ground water was derived nonrigorously from the principle of conservation of mass. The general equation relates concentration changes to hydrodynamic dispersion, convective transport, fluid sources and sinks, and chemical reactions.

Concentration changes caused by dispersion are assumed to be a function of both the dispersion coefficient and the concentration gradient. The dispersion coefficient is a second-order tensor and is related to the dispersivity of the porous medium and to the flow velocity of the ground water. If solute concentrations are affected by chemical reactions, specific mathematical expressions describing the rates of reactions must be incorporated into the general solute-transport equation.

Because both the dispersion coefficient and convective transport depend on the flow velocity, the solution of the solute-transport equation requires the definition of the velocity field, which in the general case requires that the flow and solute-transport equations be solved simultaneously. However, the solution of these equations can be considerably simplified if conditions of homogeneous fluid properties and (or) two-dimensional flow can be validly assumed.

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