measures.

An excellent text on groundwater modelling at the introductory level is Kinzelbach (1986). Huyakorn and Pinder (1983) give an advanced treatment of numerical methods with a strong mathematical basis. Luckner and Schestakow (1986) present a comprehensive survey of all types of migration processes in groundwater, with some basic numerical methods. Other texts of valuable topics include Wang and Anderson (1982), Bear and Verruijt (1987); and Molson *et al.* (in preparation).

2. REVIEW OF GOVERNING EQUATIONS

The main equations that govern the physics of groundwater flow and contaminant transport are the Darcy equation, the groundwater flow equation, and the transport equation. These are supplemented by the appropriate relationships expressing chemical and biochemical transformations.

2.1 Darcy Equation

The Darcy equation relates the flow of water through a porous medium to the driving force, which is the hydraulic gradient. In general, natural groundwater systems are anisotropic (i.e. exhibiting preferred directions of flow) due to geologic factors such as the sedimentary structure of the medium, or fracturing. In the case of anisotropy due to the sedimentary structure, flow parallel to the layering is generally favoured over flow across the layering.

The general form of the Darcy equation for three dimensional (3D) anisotropic media is (Bear, 1979; Freeze and Cherry, 1979):

$$q_x = -K_{xx}\frac{\partial\phi}{\partial x} - K_{xy}\frac{\partial\phi}{\partial y} - K_{xz}\frac{\partial\phi}{\partial z}$$

$$q_y = -K_{yx}\frac{\partial\phi}{\partial x} - K_{yy}\frac{\partial\phi}{\partial y} - K_{yz}\frac{\partial\phi}{\partial z}$$

$$q_z = -K_{zx}\frac{\partial\phi}{\partial x} - K_{zy}\frac{\partial\phi}{\partial y} - K_{zz}\frac{\partial\phi}{\partial z}$$

or in short form

$$q_i = -K_{ij}\frac{\partial\phi}{\partial x_j}$$

where $x_i = (x,y,z)$ are the coordinates of a point, q_i is the specific discharge or Darcy flux (L/T) in the direction i in the medium, K_{ij} is the hydraulic conductivity tensor (L/T), $\phi = p/\rho g + Z$ is the hydraulic head (L), with p being the pressure, ρ the density, g the gravitational acceleration, and Z the elevation head. The term $\rho g \phi$ describes the potential energy of the water at point (x,y,z). The physical meaning of a typical term in K_{ij}, say K_{xy}, is literally "the ease at which water flows in the x-direction due to a driving force acting in the y-direction". The negative sign indicates that groundwater flows toward the direction of decreasing hydraulic gradient.

When the coordinate axes are aligned parallel and perpendicular to the direction of the stratification (the principal directions of flow), a driving force applied in one of the coordinate directions will produce flow only in that direction. The Darcy equation then simplifies to:

$$q_{x'} = -K_{x'x'}\frac{\partial\phi}{\partial x'}$$

$$q_{y'} = -K_{y'y'}\frac{\partial \phi}{\partial y'}$$

$$q_{z'} = -K_{z'z'}\frac{\partial \phi}{\partial z'}$$

where (x′,y′,z′) refers to the principal directions of the medium, and $K_{i'i'}$ refers to the principal components of the hydraulic conductivity tensor.

2.2 General Groundwater Flow Equation

The flow equation is based on the continuity of fluid mass in the porous medium. The general form for heterogeneous isotropic media, without sources or sinks, is (Bear, 1979):

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial \phi}{\partial x_j}\right) = S_s\frac{\partial \phi}{\partial t}$$

where t is time, and $S_s = \rho g(\alpha + \theta\beta)$ is the specific storage of the porous medium, with θ being the porosity, α the compressibility of the porous medium, and β the compressibility of the fluid.

The above equations are valid for one-, two- and three-dimensional systems. Although most natural aquifer systems are, strictly speaking, three dimensional, 3D models require large amounts of data and are therefore applied mainly in specialized situations, or for research purposes. In practical applications, two-dimensional (2D) forms are used wherever possible. Two types of 2D models, the areal model for confined or unconfined aquifers, and the cross-sectional model for flow systems with depth-dependent processes, are in common use. The governing equations for these two types of models are discussed below.

2.3 Confined/Unconfined Aquifer Equations

If flow in an aquifer is predominantly horizontal (Fig. 1), the general 3D equation can be integrated vertically over the aquifer thickness to obtain, in the case of a confined aquifer (Bear, 1979):

$$\frac{\partial}{\partial x}\left(T\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(T\frac{\partial \phi}{\partial y}\right) - \frac{K'}{b'}\left(\phi - \phi'\right) + Q = S\frac{\partial \phi}{\partial t}$$

where T = Kb is the aquifer transmissivity, with b = b(x,y) being the aquifer thickness, S = S_sb is the aquifer storativity, K'/b'(ϕ-ϕ') represents the leakage flux from neighbouring aquifers, with K' being the vertical conductivity of the aquitard, b' being the aquitard thickness, and ϕ' the hydraulic head in the neighbouring aquifer. The term Q represents the water injected or withdrawn at wells.

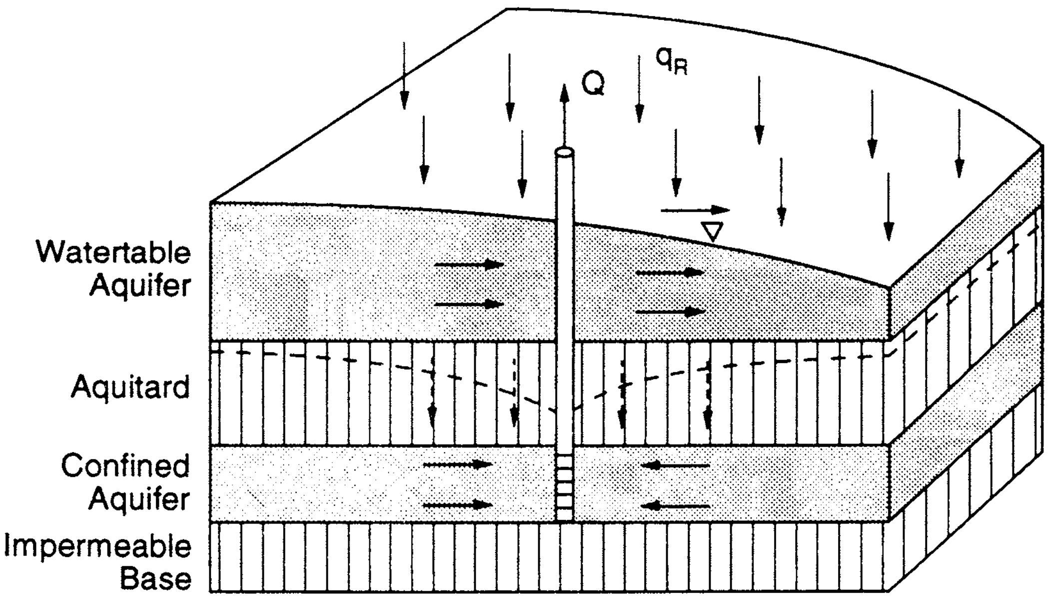

Figure 1: Confined/unconfined aquifer system

In the case of a watertable aquifer, the equation can be written as:

$$\frac{\partial}{\partial x}\left(Kb\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(Kb\frac{\partial h}{\partial y}\right) + q_R + Q = S_y\frac{\partial h}{\partial t}$$

where h is the hydraulic head at the watertable, b=h(x,y)-B(x,y) is the saturated thickness, with B being the hydraulic head at the aquifer bottom, S_y is the specific yield, and q_R is the recharge at the watertable. The watertable aquifer equation is nonlinear since the effective transmissivity Kb depends on the unknown head h through the saturated thickness b.

The boundary around the periphery of the domain (Fig. 2) should follow some identifiable natural feature. One possible feature is an open body of water such as a stream which is in contact with the aquifer, providing a fixed head (*first-type* or *Dirichlet*) boundary condition of the form:

$$\phi = h_w$$

where h_w is the hydraulic head at the boundary. An impermeable barrier (or a hydrological divide) is also a suitable boundary which provides a zero flux (*second-type* or *Neumann*) boundary condition of the form:

$$q_n = 0$$

Other possible choices are a boundary where the flux is known, or a boundary following a streamline, giving again a zero-flux boundary condition.

The basic assumptions in areal aquifer models or multi-aquifer models are:

- flow in the aquifer is essentially horizontal,
- flow in the aquitards is essentially vertical,
- storage in the aquitards is negligible.

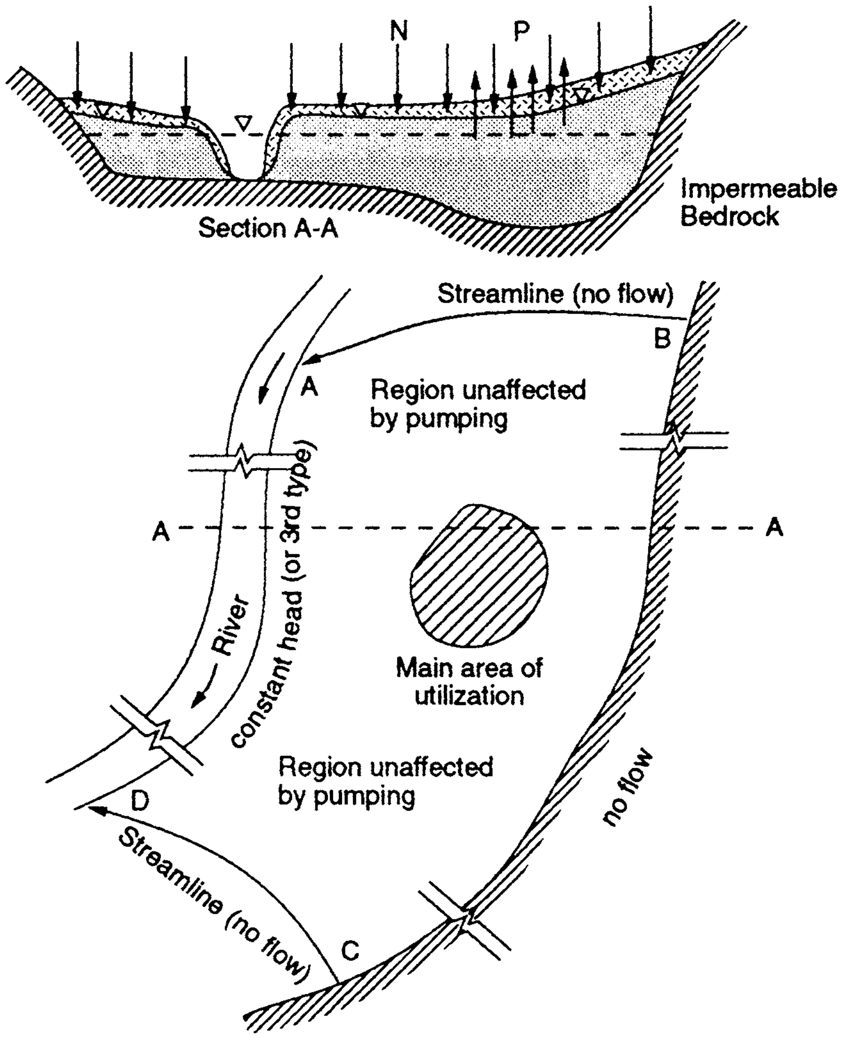

Figure 2: Boundary condition for areal flow model (modified from Bear, 1979)

These three assumptions form the basis for representing flow as 2D in the areal plane of the aquifer, and as one dimensional (1D) vertical in the aquitards with vertical flow being proportional to the head difference between the neighbouring aquifers. The validity of these assumptions must be considered when interpreting the results of 2D plan-view models. The first two assumptions are reasonable whenever the permeability contrast between the aquifers and aquitards is at least 2 orders of magnitude. The third assumption neglects the transient response in the aquitard which will normally occur when a head change is imposed in one of the aquifers. The time taken to equilibrate the system is given by (Frind, 1979):

$$t_e = \frac{S_s' \, (b')^2}{K'}$$

where S_s' is the aquitard specific storage. On the basis of this relationship, the third assumption above is reasonable if t_e is small in relation to the time period of interest.

2.4 Potential/Streamfunction Equations

Potential/streamfunction models applied in the cross-section are useful in situations where chemical or biochemical reactions play a role. Such reactions are often depth-dependent since the necessary reactants (e.g. oxygen, organic carbon, sulfides) occur at concentrations that vary with depth. Also, the reactions may be nonlinear due to the limited availability of the reactants. For these reasons, the individual transport processes cannot be averaged in the vertical over the aquifer thickness; instead, the vertical dimension must be represented explicitly in the model.

A contaminant entering the ground will first pass through the unsaturated soil zone and then enter the saturated groundwater zone. Although both of these zones can be modelled together

(Akindunni *et al.*, 1991; Akindunni and Gillham, 1992), the modelling scale is generally different. In order to stimulate unsaturated flow in a physically valid way, the soil moisture profiles must be adequately resolved in the model; this generally results in spatial discretizations of the order of centimeters. This means that, in order to keep the model manageable, its size will be restricted to a few meters (Akindunni, 1987).

In the saturated groundwater zone, on the other hand, the spatial scale of interest in contamination problems is often of the order of hundreds or thousands of meters, since both the source and the destination must be included in the model. The time scale may be of the order of several years. Therefore in problems where migration processes in the saturated zone are relevant, the unsaturated zone is often excluded. Although the flow direction in the saturated zone is predominantly horizontal, vertical velocity components are important because they can play a controlling role in chemical or biochemical reactions. We will focus here on saturated groundwater systems exclusively.

A cross-sectional flow and transport model can therefore be bounded at the top by the watertable. If the longer time scale is of interest, seasonal fluctuations are generally neglected and a long-term average flow system is assumed. The model domain can be visualized as a slice of unit thickness cut from the aquifer in the direction of groundwater flow (Fig. 3). The cut should follow the watertable gradient.

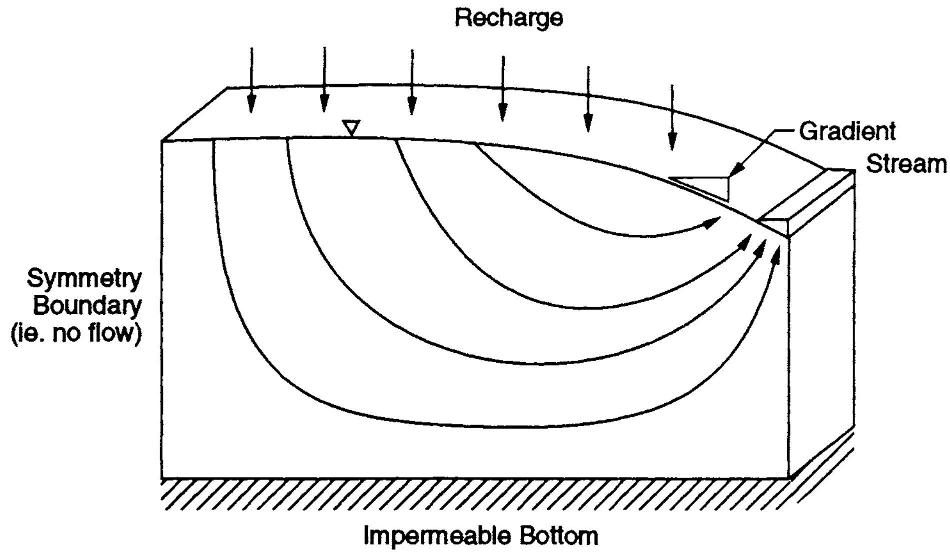

Figure 3: Typical cross-sectional flow diagram

A numerical problem can arise in cross-sectional transport modelling on account of the spatial scale. This arises because the length of the cross-sectional domain can be greater by several orders of magnitude than the width (i.e. the aquifer thickness), that is, the model domain can be very long and thin. The contrast between the horizontal and vertical scales can cause serious inaccuracies in the calculation of the groundwater velocities by means of Darcy's equation. This can in turn cause problems in the accurate definition of the flow paths that are needed in order to position the plume at the correct depth in the aquifer, and to facilitate the correct simulation of spatially dependent reactions.

This problem can be overcome by formulating the flow problem both in terms of the hydraulic potential ϕ and the streamfunction ψ. The steady-state form of the potential equation is used in this approach. The two governing equations are, in general form (Frind and Matanga, 1985):

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial \phi}{\partial x_j}\right) = 0$$

$$\frac{\partial}{\partial x_i}\left(\frac{1}{\mid K \mid}\;K_{ij}\frac{\partial \psi}{\partial x_j}\right) = 0$$

or, for the case where the coordinate axes coincide with the principal directions:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial \phi}{\partial y}\right) = 0$$

$$\frac{\partial}{\partial x}\left(\frac{1}{K_{yy}}\;\frac{\partial \psi}{\partial X}\right) + \frac{\partial}{\partial y}\left(\frac{1}{K_{xx}}\;\frac{\partial \psi}{\partial y}\right) = 0$$

where the streamfunction ψ has dimensions of discharge (L^2/T). In the above two equations, the primes to designate principal directions have been omitted.

The Darcy equation is related to the streamfunction through the relationship:

$$\begin{Bmatrix} qx \\ qy \end{Bmatrix} = -\begin{bmatrix} K_{xx} & K_{xy} \\ K_{yx} & K_{yy} \end{bmatrix}\begin{Bmatrix} \frac{\partial \phi}{\partial x} \\ \frac{\partial \phi}{\partial y} \end{Bmatrix} = \begin{Bmatrix} \frac{\partial \psi}{\partial y} \\ \frac{\partial \psi}{\partial x} \end{Bmatrix}$$

In an isotropic medium, the potential contours ϕ and the streamfunction contours (the streamlines) ψ intersect at right angles.

A useful property of the streamfunction is that the discharge in a streamtube, ΔQ, equals the streamfunction increment $\Delta\psi$ (Fig. 4). The specific discharge (Darcy velocity) is therefore:

$$q = \frac{\Delta Q}{\Delta p} = \frac{\Delta \psi}{\Delta p}$$

which is the streamfunction increment divided by the streamtube width Δp. Therefore, the streamfunction allows the determination of groundwater velocities independent of the Darcy equation. For long thin systems, streamfunction-derived velocities are usually more accurate than potential-derived velocities (Frind *et al.*, 1985).

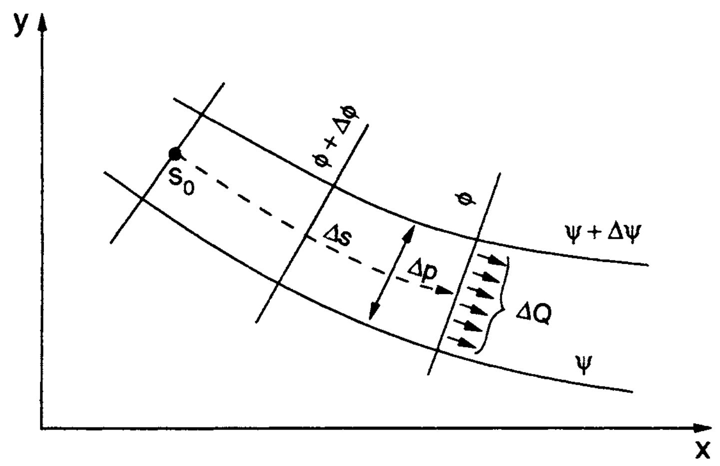

Figure 4: Streamtube in isotropic system

The streamfunction further relates the advective travel distance Δs to the travel time Δt through:

$$\Delta t = \frac{\theta}{\Delta\psi} \int_{s_o}^{s_o+\Delta s} \Delta p \; ds$$

which is simply the area of the streamtube between the points s_o and $s_o + \Delta s$, multiplied by a constant (see Fig. 4).

To solve the governing equations, boundary conditions with respect to both ϕ and ψ must be provided (Fig. 5). For the case where the location of the watertable is known, the watertable boundary condition for ϕ is:

$$\phi = h_w$$

where h_w is the watertable head. The boundary condition for ψ is expressed in terms of the component of the streamfunction gradient g_n^{ψ} in the direction normal to the boundary, which is (Frind and Matanga, 1985):

$$g_n^{\psi} = -\Delta h_w$$

Thus the normal component of the streamfunction gradient is equal to the negative rate of change of head along the watertable.

For the case where the recharge is defined at the watertable but the watertable location is unknown, the boundary condition for ψ is given in terms of the Darcy flux as:

$$q_n = q_w$$

where q_w is the specified recharge flux in the direction normal to the boundary. The boundary condition for ψ is specified in terms of the streamfunction value along the watertable, which is obtained by summing the recharge entering the system along that boundary:

$$\psi = \psi_o = \int_b q_n \, db$$

where ψ_o is a reference value, and b designates the boundary.

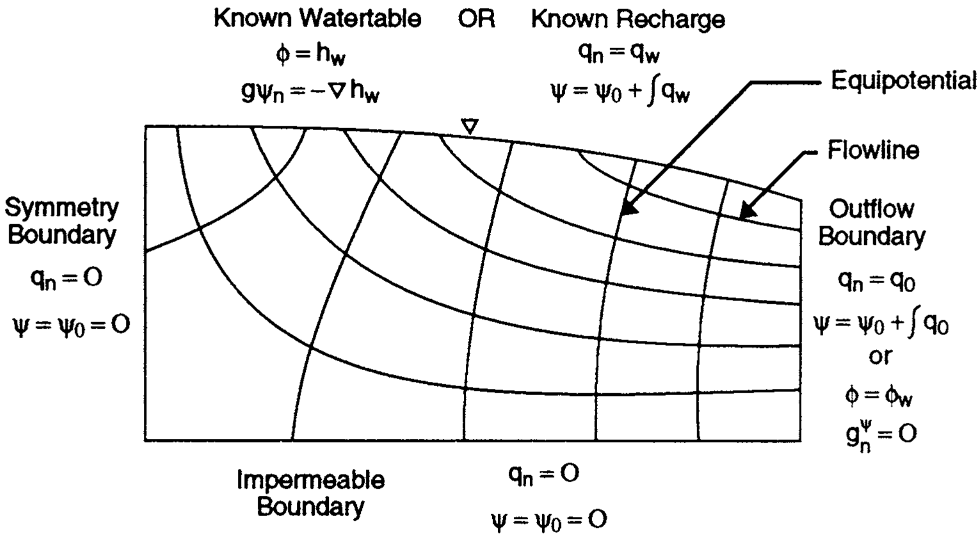

Figure 5: Boundary conditions for cross-sectional flow model

Along the bottom of the domain, we usually assume an impermeable boundary. The boundary conditions are:

$$q_n = 0$$

$$\psi = \psi_0 = 0$$

which expresses that the flux across an impermeable boundary is zero, and that the boundary is a streamline, the value of which is usually set to zero. Similar boundary conditions can be defined for the lateral boundaries.

Due to the basic assumption of flow in the plane of the cross-section, source/sink conditions such as pumping or injection wells are excluded, except when placed perpendicular to the plane of the section.

2.5 Transport Equation

The equation governing the advective-dispersive transport of a solute, subject to linear sorption and first-order decay, is (Bear, 1979; Luckner and Schestakow, 1986):

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right) - v_i\frac{\partial c}{\partial x_i} - R\lambda c = R\frac{\partial c}{\partial t}$$

where c is the concentration (usually expressed as relative with respect to the source concentration c_0, or c/c_0), D_{ij} is the dispersion tensor, $v_i = q_i/\theta$ is the average groundwater velocity, and $\lambda = \ln 2/t_{1/2}$ is the decay constant, with $t_{1/2}$ being the half-life. The retardation coefficient R is defined in standard form as (Freeze and Cherry, 1979):

$$R = 1 + \frac{\rho_b}{\theta} K_d$$

where ρ_b is the bulk density of the medium, and K_d is the linear distribution coefficient. The governing equation is based on the assumption that both the adsorbed and the dissolved phases decay. Further assumptions are that the fluid is incompressible, that there are no internal sources or sinks, and that the medium does not deform.

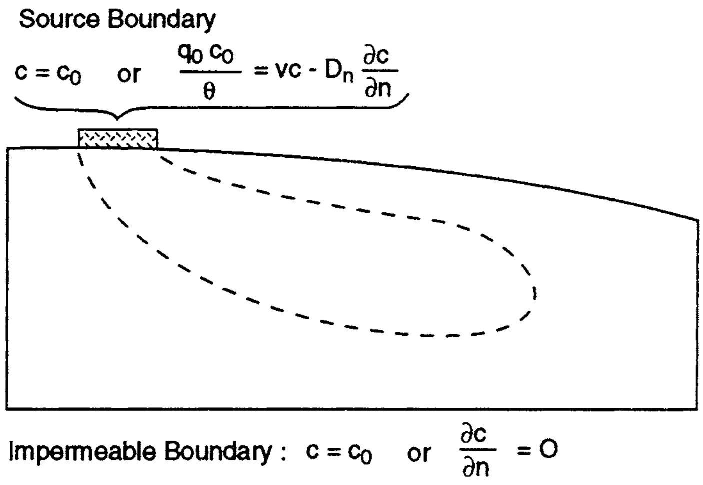

Figure 6: Boundary conditions for 2D cross-sectional transport model

The transport equation requires boundary conditions all around the domain (Fig. 6) for solution. One possible form of boundary condition is in the form of a specified concentration, which can be used in cases such as that of a waste lagoon in contact with the watertable. This gives the *first-type* or *Dirichlet* boundary condition. Alternatively, the boundary condition can be specified in the form of a known mass flux, which applies in cases such as a leaking landfill situated above the watertable where leachate is produced by rainwater percolating through the waste and the unsaturated zone to the watertable. This is known as a *third-type* or *Cauchy* boundary condition, which takes the form:

$$\frac{q_0 c_0}{\theta} = vc - D_n \frac{\partial c}{\partial n}$$

where q_0 is the known boundary recharge, c_0 is the concentration of the solute carried by the recharge water, and D_n is the dispersion coefficient in the direction normal to the boundary.

At parts of the watertable outside of the source, the above boundary condition holds with $c_0=0$. The remaining boundaries of the model (2D or 3D) are usually selected such that the contaminant does not reach the boundary. A boundary condition of either $c = 0$ or $\partial c/\partial n = 0$ (*second type* or *Neumann* boundary condition) can then be used. When a contaminant plume reaches a boundary, the correct boundary condition is the free exit boundary (Frind, 1988), which is built into the numerical solution and does not require any specified boundary values.

2.6 The Classical Concept of Dispersion

The classical definition of the 3D dispersion tensor for a medium that is isotropic with respect to dispersion is (Bear, 1979):

$$D_{ij} = \alpha_T |v| \delta_{ij} + (\alpha_L - \alpha_T) \frac{v_i v_j}{|v|} + D{*}\delta_{ij}$$

where α_L and α_T are the longitudinal and transverse dispersivities, respectively, $D^* = D_d \tau$ is the effective diffusion coefficient in the porous medium, with D_d being the molecular diffusion coefficient in solution and τ the tortuosity of the medium, and δ is the Kronecker delta. For 1D transport, this simplifies to:

$$D = \alpha_L v + D*$$

In two dimensions, the components of the symmetrical dispersion tensor take on the form:

$$D_{xx} = \alpha_L \frac{v_x^2}{|v|} + \alpha_T \frac{v_y^2}{|v|} + D*$$

$$D_{yy} = \alpha_T \frac{v_x^2}{|v|} + \alpha_L \frac{v_y^2}{|v|} + D*$$

$$D_{xy} = (\alpha_L - \alpha_T) \frac{v_x v_y}{|v|}$$

In a coordinate system following the principal directions of the dispersion tensor, which are parallel and perpendicular to the flow lines, the above components become:

$$D_{xx} = \alpha_L v + D*$$

$$D_{yy} = \alpha_T v + D*$$

$$D_{xy} = D_{xz} = D_{yz} = 0$$

The above classical definition is based on the assumption that the medium is isotropic with respect to dispersion, which means that unique values of longitudinal and transverse dispersivity can be defined for a given medium. As a consequence of that assumption, a contaminant plume would always exhibit unique spreading characteristics in the longitudinal direction as well as in the traverse direction, regardless of the direction of flow in the aquifer. We will discuss this premise further in the next section.

Figure 7 shows a typical advective-dispersive plume in 2D, based on the above theory. An analytical solution developed by Cleary and Ungs (Wexler, 1989) was used to generate the plume. The analytical solution is valid for the case of a 2D semi-infinite medium, a continuous symmetrical line source at the origin, and a first-type source boundary condition. The plume is shown both in the form of concentration contours (a), and in the form of the concentration profile at the centerline of the plume (b). The base case parameters are v=0.1m/day, α_L=1.0 m, α_T=0.1 m, R = 1.0, no decay.

In Figure 8, the parameters are varied one at a time, except for the velocity, and the resulting effect is compared with the base case. We see that increasing α_L (a) produces a typical stretching of the profile, while increasing α_T by the same proportion (b) gives a much different response due to the increased transverse spreading which depresses the profile. Doubling R reduces both the advective advance and the dispersion by one half. Introducing a decay term with $t_{1/2}$=1 year generates a profile that appears to be dominated by the exponential decay component.

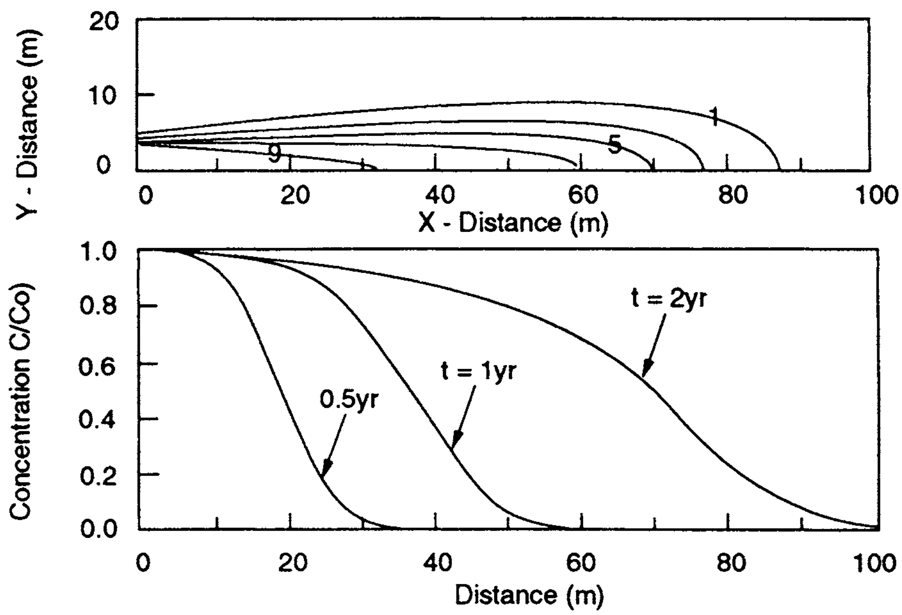

Figure 7: Advective-dispersive plume, contours and profiles

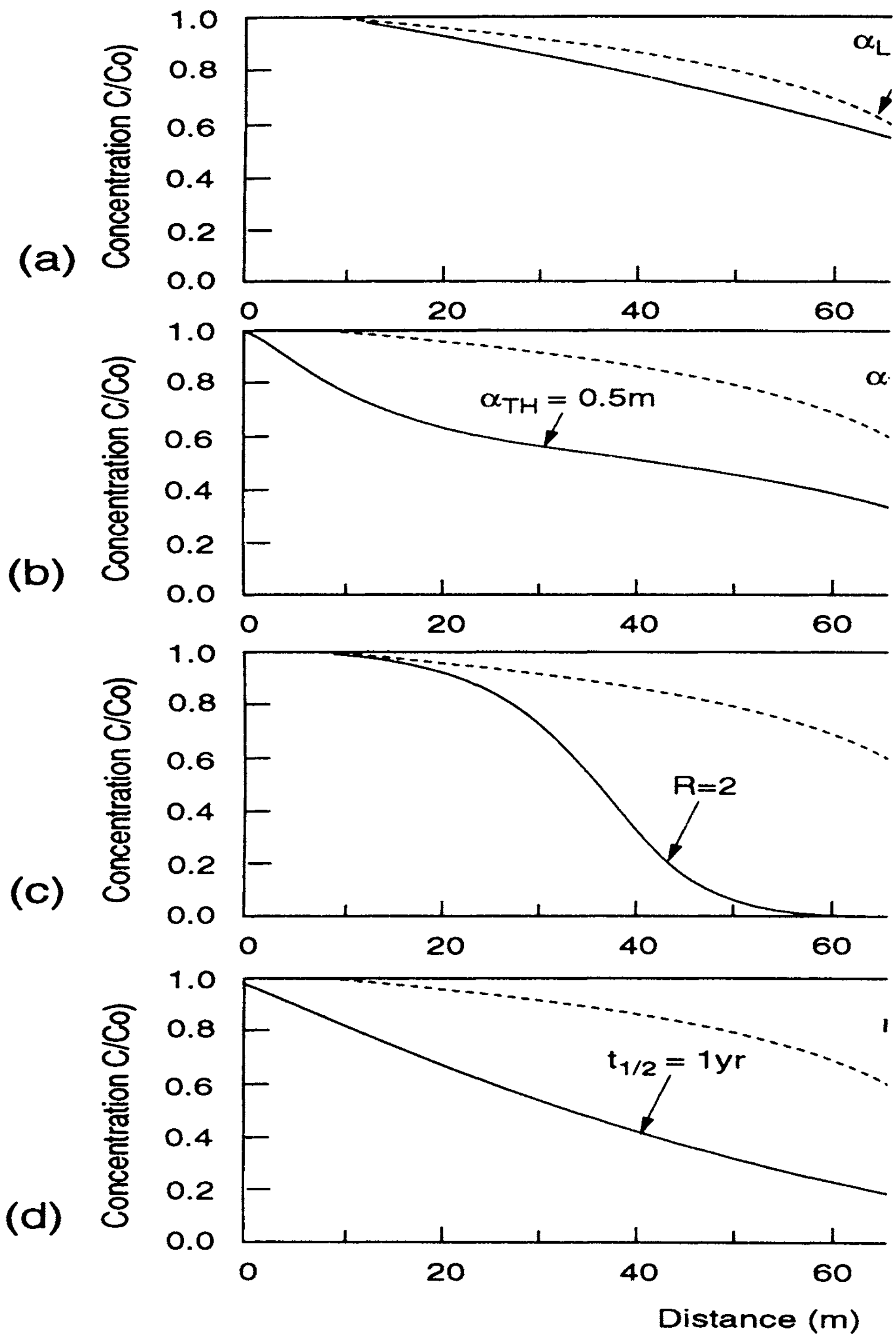

Figure 8: Advective-dispersive plume profiles at 2 years showing longitudinal, transverse dispersivity and retardation factor.

2.7 Scale-Dependent and Asymptotic Dispersion

The assumptions underlying the classical definition of dispersion are now known to be valid only at the microscale, i.e., the scale of the pores and grains in the medium. For natural heterogeneous media, it is known that transverse dispersion differs in the horizontal and vertical directions, and that the dispersivity itself may increase with scale. The scale dependence of dispersivity is a result of the heterogeneity of natural aquifer materials. As a contaminant enters the aquifer at the source, the initial dispersing mechanism is governed by the local pore-grain structure. As the contaminant migrates through the system, it progressively encounters more heterogeneities which cause the dispersing mechanism to increase. The dispersivity increases until a plateau value, the asymptotic dispersivity, is reached. Gelhar and Axness (1983) derived, on the basis of statistical analysis, expressions for the components of the asymptotic dispersivity tensor. They found that if flow is in a general direction (i.e., not parallel to the stratification), the dispersivity components are all controlled by the heterogeneity of the medium and will therefore all attain asymptotic values. For the special case where flow is parallel to the stratification, only the longitudinal dispersivity becomes asymptotic while the transverse dispersivities remain controlled by local processes.

Sudicky *et al.* (1983) showed by means of detailed field measurements that the transverse dispersivity in a natural aquifer differs in the horizontal and vertical directions. This can be explained by the differences in the sedimentary structure with respect to these directions. For the case of flow parallel to the stratification, the principal components of the asymptotic dispersion tensor can be represented as:

$$D_{xx} = (A_{11} + \alpha_L)v + D*$$

$$D_{yy} = \alpha_{TH}v + D*$$

$$D_{zz} = \alpha_{TV}v + D*$$

where α_L is the local longitudinal dispersivity, and α_{TH} and α_{TV} are the transverse horizontal and transverse vertical dispersivities, respectively. The asymptotic longitudinal dispersivity A_{11} is defined as (Gelhar and Axness, 1983):

$$A_{11} = \sigma_y^2 \frac{\lambda}{\gamma^2}$$

where σ_y^2 is the variance of the logarithm of the hydraulic conductivity, λ is the correlation length of the heterogeneities of the medium, and γ is a flow factor which was later found to be equal to 1.

Sudicky (1986) examined the spatial variability of hydraulic conductivity of a sandy aquifer in Ontario by means of highly detailed permeameter tests. He found the sand to consist of numerous thin and discontinuous lenses. He also found the hydraulic conductivity of the sand to vary over more than one order of magnitude. The resulting log conductivity variance was reported to be 0.38 and the correlation lengths of the lenses 2.8 m and 0.12 m in the horizontal and vertical directions, respectively. This study provided the first data suitable for the calculation of asymptotic dispersivities.

The asymptotic dispersivity relationships $A_{11}=\sigma_y^2\lambda$ was validated in 2D by Frind *et al.* (1987).

The physical basis of the asymptotic growth arises from the process of advective-diffusive exchange that takes place in a heterogeneous medium consisting of lenses having higher and lower values of hydraulic conductivity. In such a medium, a solute will advance advectively faster in a high-conductive zone and the resulting concentration gradient between high- and low-conductive zones will give rise to transverse diffusive transport. Mass is thus removed from the front of the plume and stored temporarily in the low-conductive layers. When the plume has passed the low-conductive zone, the concentration gradient reverses and the mass moves back into the high-conductive zone to be added to the tail end of the plume. In an aquifer containing many of these zones of differing conductivity, the aggregate of these mass exchanges, seen over the system as a whole, results in an apparent growth of the overall dispersivity. Eventually, the process stabilizes at the level of the asymptotic dispersivity. The study also confirmed that the transverse vertical dispersivity remains at its local value.

The dispersivity reaches its asymptotic value at a travel distance of about 40-50 correlation lengths from the source (Frind *et al.*, 1987). For pre-asymptotic conditions, unfortunately, rigorously valid scale-dependent dispersivity relationships that are easy to implement in numerical models have not yet been developed. Although the microscale approach is valid, its cost renders it impractical in normal situations. A dilemma therefore arises in the modelling of advective-dispersive transport in the pre-asymptotic range. One possible option may be to select an empirical dispersivity function that takes on a local value at the source and grows to the required asymptotic value. Fortunately, field problems may not be overly sensitive to the precise value of the dispersivity as long as it is in the correct range (Frind and Molson, 1989).

3. SOLUTION OF SIMULTANEOUS EQUATIONS

Numerical solutions of problems in groundwater studies create systems of simultaneous equations which could be very large. The number of unknown parameters in these equations are often between 100 and 1000, sometimes up to one million. The equations are also generally banded. Efficient techniques are required to solve these equations. The equations