boundaries until the water levels predicted by the model were similar to observed data. The calibrated model was then used to determine the effect of a hydraulic trap in the form of a purge well which was intended to provide protection against contamination from the collector well.

Another study is presented in Appendix 3 where finite elements method was used to investigate a concept that would ordinarily be difficult to demonstrate. A 1D saturated-unsaturated flow model was applied to the transient drainage of water through a two-layer vertical column of porous media. The objective was to demonstrate the hydraulic principles involved in the use of fine-grained materials as protective covers for reactive mine tailings. The objective of installing the covers is to keep the materials at high moisture content thereby reducing the influx of oxygen into the reactive tailings. In the study provided in Appendix 3, emphasis was placed on the choice of materials which have appropriate physical properties to achieve the set objectives because of the dependence of observed response of the two-layer system on the retention characteristics of the component materials. The study further demonstrates how models could be used for the purpose of system design.

6. PARTICLE TRACKING METHODS

Particle tracking methods offer a valuable alternative to finite difference and finite element methods for simulating contaminant transport. In particle tracking, the distribution of a solute in the groundwater is represented by a finite number of particles, where each particle carried either a certain concentration or a certain fraction of the total mass. The particles are moved through the domain according to the velocity field, and their behaviour is observed. The status of the system at a given time can be deduced from the distribution of the particles. The accuracy and smoothness of the solution will depend on the number of particles used.

One of the main advantages of particle tracking is that the Peclet constraint on the grid spacing does not apply and that the type of numerical dispersion that is controlled by this

constraint does not occur. The method is therefore well-suited for advection-dominated problems, where the Peclet constraint would dictate a very fine spacial discretization if finite difference or finite element methods were applied. Freedom from the Peclet constraint, however, does not mean that the spatial discretization can be indiscriminately large since the accuracy of the final solution still depends on the grid resolution.

Before solving the transport equation by either finite differences, finite elements, or particle tracking, the velocity field must first be determined. This is usually accomplished by numerically differentiating the hydraulic heads obtained from the numerical solution of the flow equation. A major difference between finite elements and particle tracking lies in the manner in which the flow velocities are used in the transport calculations: In finite elements, velocities are used in an integrated form, while in particle tracking, they are used directly for advecting the particles. For this reason, element-wise discontinuous velocities are not acceptable in particle tracking. Sophisticated interpolation procedures are therefore used in order to obtain a continuous velocity field (Kinzelbach, 1986). The relative ease of implementation of these interpolation procedures when using rectangular grids leads to a preference for finite difference methods for the calculation of the heads in most particle tracking schemes.

A disadvantage of particle tracking is that nonlinear chemical or biochemical processes are not easily incorporated. The optimal use of particle tracking methods is thus in hydraulically-oriented situations, such as pump-and-treat remediation measures for groundwater contamination, or the delineation of groundwater protection zones. In purging situations, the key question to be addressed often concerns the optimal strategy for the hydraulic removal of a contaminant plume from the aquifer. Dispersion is of secondary importance in such cases.

6.1 The Method of Characteristics

One of the most popular transport codes today is the Method of Characteristics (MOC) code developed by Konikow and Bredehoeft (1978). To understand the method, the transport

process can be conveniently visualized by considering a single particle. The particle is carried along by the moving water and it experiences dispersion, sorption, and decay along the way. These processes are all linear and they can therefore be considered separately and superimposed. The particle is considered to be representative of some control volume and it is accordingly tagged with an initial concentration equivalent to the average concentration of that control volume. The particle moves along *pathlines* (the characteristic curves) in the velocity field (Fig. 29).

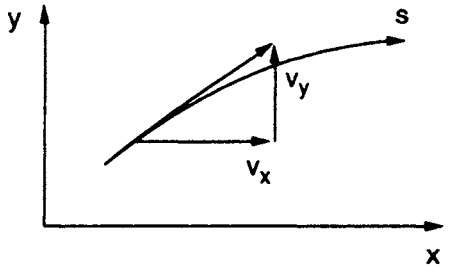

Figure 29: Pathline in 2D flow field

In two dimensions, the rate of change of concentration in the moving particle is given by the *substantial derivative*:

$$\frac{dc}{dt} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x}\frac{dx}{dt} + \frac{\partial c}{\partial y}\frac{dy}{dt}$$

where the first term on the right-hand side represents the changes experienced by the moving particle and the remaining terms represent the changes due to the motion of the particle. The *characteristic equations* are:

$$\frac{dx}{dt} = v_x$$

and

$$\frac{dy}{dt} = v_y$$

where v_x,v_y represent the velocity components. The above equations are known as the incompressible form of the *Euler equations*. In the absence of sources or sinks and no dispersion or decay, we have:

$$\frac{\partial c}{\partial t} = v_x\frac{\partial c}{\partial x} + v_y\frac{\partial c}{\partial y} = 0$$

so that:

$$\frac{dc}{dt} = 0$$

Therefore, the concentration of the moving particle will remain the same in the non-dispersive and non-reactive case. The displacement of the particle up to time t is expressed exactly by integrating along the pathline equation:

$$x(t)=x_0 + \int_{t_0}^{t} v_x(x(\tau),y(\tau))d\tau$$

$$y(t) = y_0 + \int_{t_0}^{t} v_y(x(\tau),y(\tau))d\tau$$

where x_0, y_0, t_0 are the starting point and time, and τ is the integration variable. In the numerical solution, the finite displacement during the time interval from t to t+Δt is

determined by performing an equivalent but approximate numerical integration (Fig. 30):

$$x(t+\Delta t) = x(t) + v_x(x(t),y(t))\Delta t$$

$$y(t+\Delta t) = y(t) + v_y(x(t),y(t))\Delta t$$

Since the velocity at the starting point is used here, the calculation represents an explicit (upstream) approximation, which is first-order accurate. Alternatively, center-weighted procedures can be used that iteratively calculate the advective displacement in terms of the average of the velocities at the old and new positions, giving second-order accuracy.

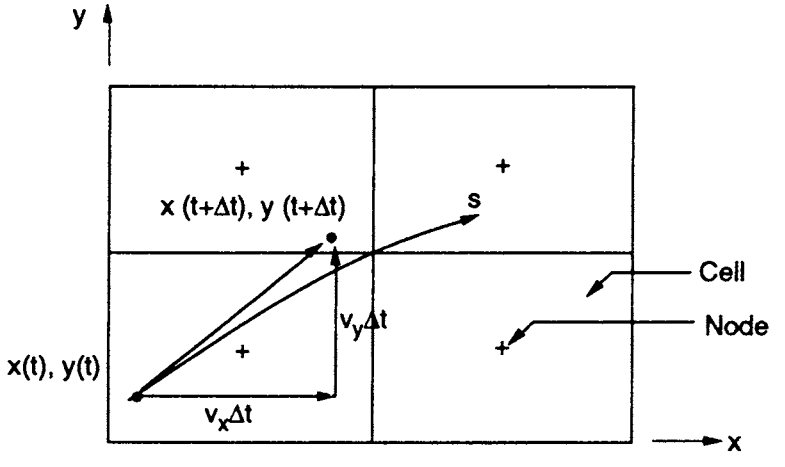

Figure 30: Advective displacement of a particle

The processes of dispersion, decay, and retardation can be considered separately in the MOC. If dispersion were to occur in addition to advection, the term expressing the change of concentration of the moving particle (see substantial derivative equation) will become:

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

which is the pure-dispersion equation for the moving particle.

Since dispersion is a process that redistributes mass, the solution of the above equation requires consideration of all particles together. The solution is analogous to the procedure discussed in Section 3.2. For example, for a uniformly-spaced grid where the coordinate axes coincide with the principal directions of the dispersion tensor, the explicit calculation will yield a dispersive change over the time step Δt at particle location i,j (Fig. 31) given by:

$$\Delta c_{i,j} = c(t+\Delta t)_{i,j} - c(t)_{i,j} = \Delta t\, D_{xx}\left\{\frac{c_{i-1,j} - 2c_{i,j} + c_{i+1,j}}{(\Delta x)^2}\right\}_t + \Delta t D_{yy}\left\{\frac{c_{i,j-1} - 2c_{i,j} + c_{i,j+1}}{(\Delta y)^2}\right\}_t$$

where the right-hand side is entirely in terms of the concentrations at the old time level. A more general procedure valid for an arbitrary coordinate orientation and variable coefficients, which requires 9 nodal points for the calculation of $\Delta c_{i,j}$, is discussed by Kinzelbach (1986). In order to obtain the regular grid pattern required for the dispersive calculation, the particles must be reassigned (with suitable concentration adjustments) to the cell centers prior to the dispersive calculation.

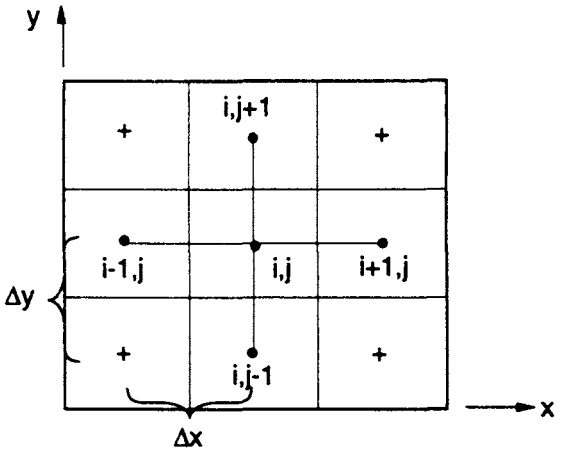

Figure 31: Particle pattern for explicit calculation of dispersive transport component

The above explicit calculation is subject to the stability constraint:

$$\Delta t \left(\frac{D_{xx}}{(\Delta x)^2} + \frac{D_{yy}}{(\Delta y)^2} \right) \leq \frac{1}{2}$$

Alternatively, an implicit solution procedure can be used which avoids the stability constraint. Konikow and Bredehoeft (1978) use the explicit procedure.

Decay is a process that operates on each particle individually. The change experienced by the moving particle is in that case given by:

$$\frac{\partial c}{\partial t} = -\lambda c$$

and the finite change Δc over the time step Δt is accordingly:

$$\Delta c = c(t+\Delta t) - c(t) = -\lambda c(t)\Delta t$$

The change calculated for each particle is added to the existing particle concentration.

Linear sorption can be incorporated easily by dividing the velocity v and the dispersion coefficient D by the retardation coefficient (R), which is given by:

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

The effect of this process will be a slowing down of the advective advance and the spreading.

Observance of the grid Courant constraint is necessary in all particle tracking procedures in order to limit particle migration to no more than one cell length per time step. If this constraint were exceeded, particles would literally jump across intervening cells, and the information resident in those cells would remain unused. This constraint is independent of the stability constraint that applies to the explicit solution of the dispersive transport component. Although a formal constraint on the grid spacing, analogous to the Peclet constraint, does not exist in particle tracking methods, the grid spacing nevertheless controls the resolution of the velocity field, and hence the accuracy of the simulation. Therefore, a reasonably fine cell spacing should be used in areas of large gradient changes. If dispersion is included, particles must be distributed throughout the domain, including areas that initially have zero concentration, to allow for the spreading of the plume.

6.2 Capture Zones and Plume Purging

The travel time T of a particle along its pathline can be computed easily by accumulating the time steps:

$$T = \sum_k \Delta t_k$$

By releasing particles along a contaminant front and recording their position at specified time levels, the advective advance of a front can be displayed at different times.

A useful concept in groundwater protection is the *capture zone* of a well, which is defined as the zone within which all water is eventually captured by the well. A capture zone can be generated by starting a number of particles around the periphery of the well and tracking them in the reverse flow direction. The capture zone is time-dependent and it will continue to expand until the withdrawal at the well is balanced by recharge from the surface, from neighbouring aquifers, or from the boundaries. If the well is a water supply well, the capture zone will define the zone that is sensitive to contamination and that may be designated as a *groundwater protection zone*. Figure 32 shows typical time-related capture zones associated with a single pumping well in a uniform flow field for 3 different points in time.

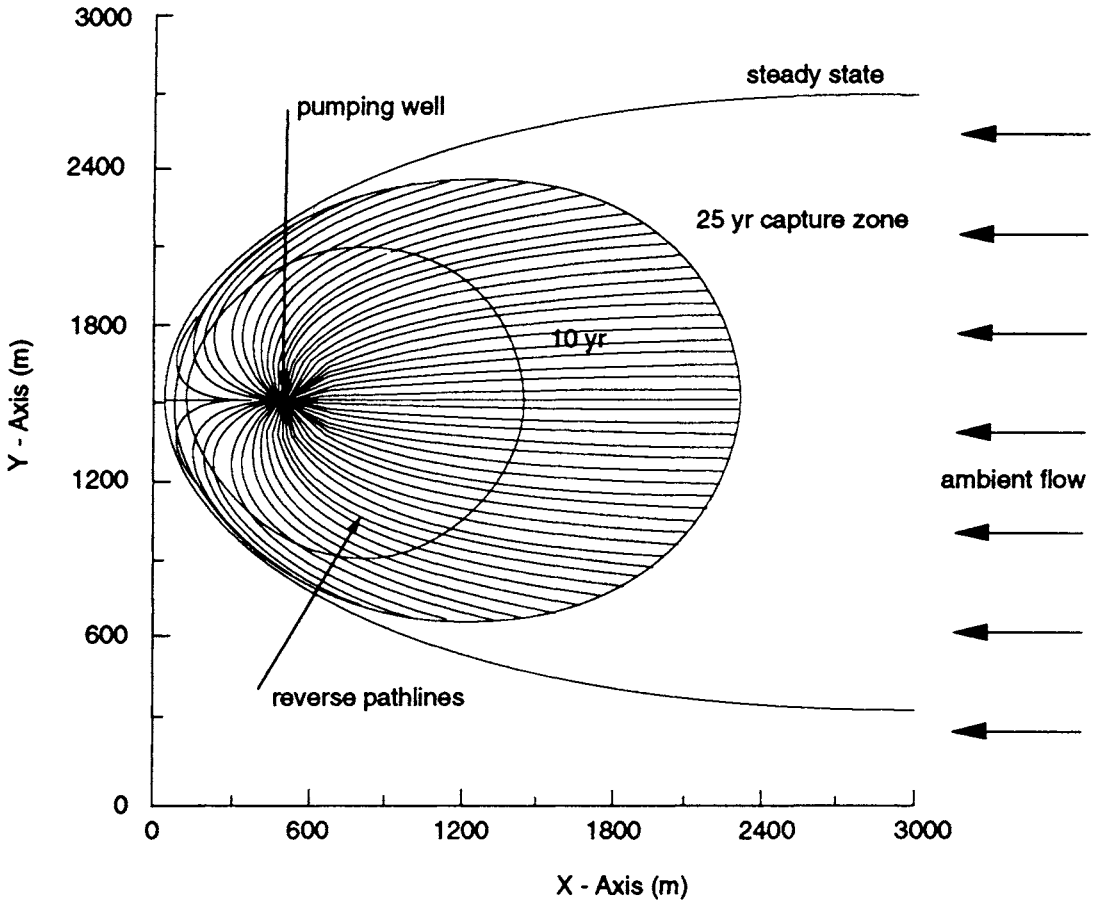

Figure 32: Pathlines and capture zones in a uniform flow field

The capture zone concept is also useful in the context of hydraulic purging of groundwater contamination. If the extent of contamination is known, the purge well can be placed in such

a way that its capture zone encompasses the plume. The purging operation can then be simulated by tracking the particles representing the boundary of the capture zone back to the well. Questions such as the optimal location of the purge well or wells, and the time required for plume removal, are usually of prime interest in the planning of the operation.

In the case of plume purging, the plume will be in a condition of maximal dispersal prior to purging. The additional dispersion occurring during the purge operation is therefore of little interest and the dispersive transport component can be justifiably neglected. Linear adsorption/desorption as well as first-order decay may be of interest and can be included. Overall, however, the most important transport component in such situations is the advective component. The MOC, in its advective mode, is therefore well suited for handling such situations.

One aspect that may play a role in plume purging is the fact that contaminant mass can be retained in low-conductivity zones within a heterogeneous aquifer. Thus a significant portion of the mass may still be in the aquifer even though the hydraulic remediation would indicate complete removal of the plume. This is known as the *dual porosity* phenomenon, which, unfortunately, is not easily incorporated into the MOC.

6.3 The Random Walk Method

The Random Walk Method (Prickett *et al.*, 1981) differs from the MOC in that each particle represents a fixed mass, so that the sum of all particle masses equals the total mass in the system. Particles are displaced advectively and dispersively. For simplicity, we will here consider a 1D system. In this case, the advective-dispersive displacement of a particle with respect to its initial position is given by (Fig. 33):

$$v = vt + \rho\sqrt{2Dt}$$

where $\rho \sim N(0,1)$ is a normally-distributed random variable with mean = 0 and standard deviation = 1, and where $D = \alpha v$. The random variable ρ is obtained from a random number generator.

The time stepping scheme for the 1D problem therefore becomes:

$$x(t+\Delta t) = x(t) + v\Delta t + \rho\sqrt{2\alpha v\Delta t}$$

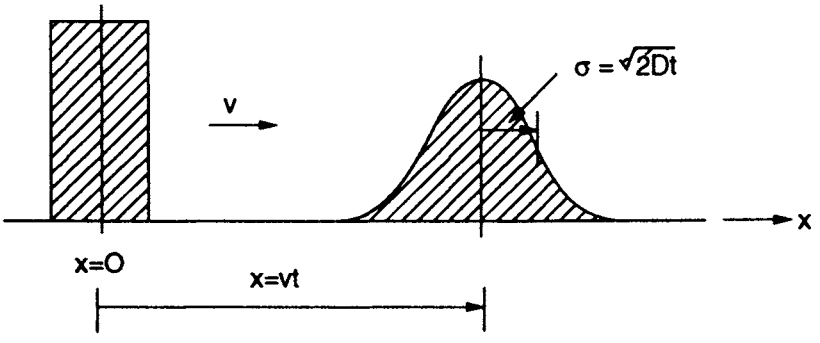

Figure 33: Advective-dispersive displacement in Random Walk Method

This is again an explicit procedure having first-order accuracy. The corresponding 2D formulation is similar.

A problem arises here (Kinzelbach, 1986) in that the advective-dispersive displacement calculated by the above equation represents a solution not to the advection-dispersion equation:

$$\frac{\partial c}{\partial t} + \frac{\partial (vc)}{\partial x} - \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) = 0$$

but to the slightly different equation:

$$\frac{\partial c}{\partial t} + \frac{\partial (vc)}{\partial x} - \frac{\partial^2 (Dc)}{\partial x^2} = 0$$

In order to amend this discrepancy, a correction is added to the velocity term giving:

$$v^*(x,t) = v(x,t) + \frac{\partial D(x,t)}{\partial x}$$

The correction $\partial D/\partial x$ is applied whenever the dispersion coefficient $D=\alpha v$ varies on account of either a variable velocity or a variable dispersivity or both. The corrected velocity v^* is used in the calculation of the advective displacement.

A scale-dependent dispersivity can be incorporated in the random walk method by utilizing some suitable function that would take on the value of the local dispersivity at the source, and that would increase asymptotically to the field value over a travel distance of about 40 to 50 correlation lengths of the statistically homogeneous medium. Linear sorption and first-order decay can also be incorporated in the same way as in the MOC.

The number of particles required in the Random Walk Method is controlled primarily by the requirement to have a sufficient number of particles left in low-concentration zones (the fringes of the plume) for the calculation of concentrations. Thus the anticipated dispersion, retardation, and decay mechanisms must be considered when selecting particle populations.