Techniques of Water-Resources Investigations of the United States Geological Survey

Chapter C2

COMPUTER MODEL OF TWO-DIMENSIONAL SOLUTE TRANSPORT AND DISPERSION IN GROUND WATER

By L. F. Konikow and J. D. Bredehoeft

Book 7

AUTOMATED DATA PROCESSING AND COMPUTATIONS

DEPARTMENT OF THE INTERIOR

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PREFACE

The series of manuals on techniques describes procedures for planning and executing specialized work in water-resources investigations. The material is grouped under major headings called books and further subdivided into sections and chapters; section C of Book 7 is on computer programs.

This chapter presents a digital computer model for calculating changes in the concentration of a dissolved chemical species in flowing ground water. The computer program represents a basic and general model that may have to be modified by the user for efficient application to his specific field problem. Although this model will produce reliable calculations for a wide variety of field problems, the user is cautioned that in some cases the accuracy and efficiency of the model can be affected significantly by his selection of values for certain user-specified options.

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COMPUTER MODEL OF TWO-DIMENSIONAL SOLUTE TRANSPORT AND DISPERSION IN GROUND WATER

By L. F. Konikow and J. D. Bredehoeft

Abstract

This report presents a model that simulates solute transport in flowing ground water. The model is both general and flexible in that it can be applied to a wide range of problem types. It is applicable to one- or two-dimensional problems involving steady-state or transient flow. The model computes changes in concentration over time caused by the processes of convective transport, hydrodynamic dispersion, and mixing (or dilution) from fluid sources. The model assumes that the solute is nonreactive and that gradients of fluid density, viscosity, and temperature do not affect the velocity distribution. However, the aquifer may be heterogeneous and (or) anisotropic.

The model couples the ground-water flow equation with the solute-transport equation. The digital computer program uses an alternating-direction implicit procedure to solve a finite-difference approximation to the ground-water flow equation, and it uses the method of characteristics to solve the solute-transport equation. The latter uses a particle-tracking procedure to represent convective transport and a two-step explicit procedure to solve a finite-difference equation that describes the effects of hydrodynamic dispersion, fluid sources and sinks, and divergence of velocity. This explicit procedure has several stability criteria, but the consequent time-step limitations are automatically determined by the program.

The report includes a listing of the computer program, which is written in FORTRAN IV and contains about 2,000 lines. The model is based on a rectangular, block-centered, finite-difference grid. It allows the specification of any number of injection or withdrawal wells and of spatially varying diffuse recharge or discharge, saturated thickness, transmissivity, boundary conditions, and initial heads and concentrations. The program also permits the designation of up to five nodes as observation points, for which a summary table of head and concentration versus time is printed at the end of the calculations. The data input formats for the model require three data cards and from seven to nine data sets to describe the aquifer properties, boundaries, and stresses.

The accuracy of the model was evaluated for two idealized problems for which analytical solutions could be obtained. In the case of one-dimensional flow the agreement was nearly exact, but in the case of plane radial flow a small amount of numerical dispersion occurred. An analysis of several test problems indicates that the error in the mass balance will be generally less than 10 percent. The test problems demonstrated that the accuracy and precision of the numerical solution is sensitive to the initial number of particles placed in each cell and to the size of the time increment, as determined by the stability criteria. Mass balance errors are commonly the greatest during the first several time increments, but tend to decrease and stabilize with time.

Introduction

This report describes and documents a computer model for calculating transient changes in the concentration of a nonreactive solute in flowing ground water. The computer program solves two simultaneous partial differential equations. One equation is the ground-water flow equation, which describes the head distribution in the aquifer. The second is the solute-transport equation, which describes the chemical concentration in the system. By coupling the flow equation with the solute-transport equation, the model can be applied to both steady-state and transient flow problems.

The purpose of the simulation model is to compute the concentration of a dissolved chemical species in an aquifer at any specified place and time. Changes in chemical concentration occur within a dynamic ground-water system primarily due to four distinct processes: (1) convective transport, in which dissolved chemicals are moving with the flowing ground water; (2) hydrodynamic dispersion, in which molecular and ionic diffusion and small-scale variations in the velocity of flow through the porous media cause the paths of dissolved molecules and ions to diverge or spread from the average direction of ground-water flow; (3) fluid sources, where water of one composition is introduced into water of a different composition; and (4) reactions, in which some amount of a particular dissolved chemical species may be added to or removed from the ground water due to chemical and physical reactions in the water or between the water and the solid aquifer materials. The model presented in this report assumes (1) that no reactions occur that affect the concentration of the species of interest, and (2) that gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.

This model can be applied to a wide variety of field problems. However, the user should first become aware of the assumptions and limitations inherent in the model, as described in this report. The computer program presented in this report is offered as a basic working tool that may have to be modified by the user for efficient application to specific field problems. The program is written in FORTRAN IV and is compatible with most high-speed computers. The data requirements, input format specifications, program options, and output formats are all structured in a general manner that should be readily adaptable to many field problems.

This report includes a detailed description of the numerical method used to solve the solute-transport equation. The reader is assumed to have (or can obtain elsewhere) a moderate familiarity with finite-difference methods and ground-water flow models.

Theoretical Background

Flow equation

By following the derivation of Pinder and Bredehoeft (1968), the equation describing the transient two-dimensional areal flow of a homogeneous compressible fluid through a nonhomogeneous anisotropic aquifer can be written in Cartesian tensor notation as

$$\frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial h}{\partial x_j}\right)=S\frac{\partial h}{\partial t}+W \qquad i,j=1,2 \qquad (1)$$

where

- T_{ij} is the transmissivity tensor, L^2/T;
- h is the hydraulic head, L;
- S is the storage coefficient, (dimensionless);
- t is the time, T;
- $W=W(x,y,t)$ is the volume flux per unit area (positive sign for outflow and negative for inflow), L/T; and
- x_i and x_j are the Cartesian coordinates, L.

If we only consider fluxes of (1) direct withdrawal or recharge, such as well pumpage, well injection, or evapotranspiration, and (2) steady leakage into or out of the aquifer through a confining layer, streambed, or lakebed, then $W(x,y,t)$ may be expressed as

$$W(x,y,t)=Q(x,y,t)-\frac{K_z}{m}(H_s-h) \qquad (2)$$

where

- Q is the rate of withdrawal (positive sign) or recharge (negative sign), L/T;
- K_z is the vertical hydraulic conductivity of the confining layer, streambed, or lakebed, L/T;
- m is the thickness of the confining layer, streambed, or lakebed, L; and
- H_s is the hydraulic head in the source bed, stream, or lake, L.

Lohman (1972) shows that an expression for the average seepage velocity of ground water can be derived from Darcy's law. This expression can be written in Cartesian tensor notation as

$$V_i=-\frac{K_{ij}}{\epsilon}\frac{\partial h}{\partial x_j} \qquad (3)$$

where

- V_i is the seepage velocity in the direction of x_i, L/T;
- K_{ij} is the hydraulic conductivity tensor, L/T; and
- ϵ is the effective porosity of the aquifer, (dimensionless).

Transport equation

The equation used to describe the two-dimensional areal transport and dispersion of a given nonreactive dissolved chemical species in flowing ground water was derived by Reddell and Sunada (1970), Bear (1972), Bredehoeft and Pinder (1973), and Konikow and Grove (1977). The equation may be written as

$$\frac{\partial(Cb)}{\partial t}=\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right)-\frac{\partial}{\partial x_i}(bCV_i)-\frac{C'W}{\epsilon}\qquad i,j=1,2 \quad (4)$$

where

- C is the concentration of the dissolved chemical species, M/L^3;
- D_{ij} is the coefficient of hydrodynamic dispersion (a second-order tensor), L^2/T;
- b is the saturated thickness of the aquifer, L; and
- C' is the concentration of the dissolved chemical in a source or sink fluid, M/L^3.

The first term on the right side of equation 4 represents the change in concentration due to hydrodynamic dispersion. The second term describes the effects of convective transport, while the third term represents a fluid source or sink.

Dispersion coefficient

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 dispersion coefficient may be related to the velocity of ground-water flow and to the nature of the aquifer using Scheidegger's (1961) equation:

$$D_{ij}=\alpha_{ijmn}\frac{V_mV_n}{|V|} \quad (5)$$

where

- α_{ijmn} is the dispersivity of the aquifer, L;
- V_m and V_n are components of velocity in the m and n directions, respectively, L/T; and
- $|V|$ is the magnitude of the velocity, L/T.

Scheidegger (1961) further shows that for an isotropic aquifer the dispersivity tensor can be defined in terms of two constants. These are the longitudinal and transverse dispersivities of the aquifer (α_L and α_T, respectively). These are related to the longitudinal and transverse dispersion coefficients by

$$D_L=\alpha_L|V| \quad (6)$$

and

$$D_T=\alpha_T|V|. \quad (7)$$

After expanding equation 5, substituting Scheidegger's identities, and eliminating terms with coefficients that equal zero, the components of the dispersion coefficient for two-dimensional flow in an isotropic aquifer may be stated explicitly as

$$D_{xx}=D_L\frac{(V_x)^2}{|V|^2}+D_T\frac{(V_y)^2}{|V|^2}; \quad (8)$$

$$D_{yy}=D_T\frac{(V_x)^2}{|V|^2}+D_L\frac{(V_y)^2}{|V|^2}; \quad (9)$$

$$D_{xy}=D_{yx}=(D_L-D_T)\frac{V_xV_y}{|V|^2}. \quad (10)$$

Note that while D_{xx} and D_{yy} must have positive values, it is possible for the cross-product terms (eq 10) to have negative values if V_x and V_y have opposite signs.

Review of assumptions

A number of assumptions have been made in the development of the previous equations. Following is a list of the main assumptions that must be carefully evaluated before applying the model to a field problem.

1. Darcy's law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow.
2. The porosity and hydraulic conductivity of the aquifer are constant with time, and porosity is uniform in space.
3. Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
4. No chemical reactions occur that affect the concentration of the solute, the fluid properties, or the aquifer properties.
5. Ionic and molecular diffusion are negligible contributors to the total dispersive flux.
6. Vertical variations in head and concentration are negligible.
7. The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

The nature of a specific field problem may be such that not all of these underlying assumptions are completely valid. The degree to which field conditions deviate from these assumptions will affect the applicability and reliability of the model for that problem. If the deviation from a particular assumption is significant, the governing equations will have to be modified to account for the appropriate processes or factors.

Numerical Methods

Because aquifers have variable properties and complex boundary conditions, exact analytical solutions to the partial differential equations of flow (eq 1) and solute transport (eq 4) cannot be obtained directly. Therefore, approximate numerical methods must be employed.

The numerical methods require that the area of interest be subdivided by a grid into a number of smaller subareas. The model developed here utilizes a rectangular, uniformly spaced, block-centered, finite-difference grid, in which nodes are defined at the centers of the rectangular cells.

Flow equation

Pinder and Bredehoeft (1968) show that if the coordinate axes are alined with the principal directions of the transmissivity tensor, equation 1 may be approximated by the following implicit finite-difference equation:

$$\begin{aligned} T_{xx[i-\frac{1}{2},j]}\left[\frac{h_{i-1,j,k}-h_{i,j,k}}{(\Delta x)^2}\right] &+T_{xx[i+\frac{1}{2},j]}\left[\frac{h_{i+1,j,k}-h_{i,j,k}}{(\Delta x)^2}\right] \\ &+T_{yy[i,j-\frac{1}{2}]}\left[\frac{h_{i,j-1,k}-h_{i,j,k}}{(\Delta y)^2}\right] \\ &+T_{yy[i,j+\frac{1}{2}]}\left[\frac{h_{i,j+1,k}-h_{i,j,k}}{(\Delta y)^2}\right] \\ =S\left[\frac{h_{i,j,k}-h_{i,j,k-1}}{\Delta t}\right] &+\frac{q_{w(i,j)}}{\Delta x\Delta y}\;\frac{K_z}{m}[H_{s(i,j)}-h_{i,j,k}] \end{aligned} \quad (11)$$

where

- i,j,k are indices in the x, y, and time dimensions, respectively;
- $\Delta x,\Delta y,\Delta t$ are increments in the x, y, and time dimensions, respectively; and
- q_w is the volumetric rate of withdrawal or recharge at the (i,j) node, L^3/T.

Note that k represents the new time level and k–1 represents the previous time level. To avoid confusion between tensor subscripts and nodal indices, the latter are separated by commas.

The finite-difference equation (eq 11) is solved numerically for each node in the grid using an iterative alternating-direction implicit (ADI) procedure. The derivation and solution of the finite-difference equation and the use of the iterative ADI procedure have been previously discussed in detail in the literature. Some of the more relevant references include Pinder and Bredehoeft (1968), Prickett and Lonnquist (1971), and Trescott, Pinder, and Larson (1976).

After the head distribution has been computed for a given time step, the velocity of ground-water flow is computed at each node using an explicit finite-difference form of equation 3. For example, the velocity in the x direction at node (i,j) would be computed as

$$V_{x(i,j)}=\frac{K_{xx(i,j)}}{\epsilon}\frac{(h_{i-1,j,k}-h_{i+1,j,k})}{2\Delta x}. \quad (12)$$

The velocity in the x direction can also be computed on the boundary between node (i,j) and node $(i+1,j)$ using the following equation:

$$V_{x(i+½,j)}=\frac{K_{xx(i+½,j)}}{\epsilon}\frac{(h_{i,j,k}-h_{i+1,j,k})}{\Delta x} \quad (13)$$

where the hydraulic conductivity on the boundary is computed as the harmonic mean of the hydraulic conductivities at the two adjacent nodes.

Expressions similar to equations 12 and 13 are used to compute the velocities in the y direction at (i,j) and $(i,j+½)$ respectively. Note that equation 13, which computes the head difference over a distance Δx, is more accurate than equation 12, which computes the head difference over $2\Delta x$.

Transport equation

Method of characteristics

The method of characteristics is used in this model to solve the solute-transport equation. This method was developed to solve hyperbolic differential equations. If solute transport is dominated by convective transport, as is common in many field problems, then equation 4 may closely approximate a hyperbolic partial differential equation and be highly compatible with the method of characteristics. Although it is difficult to present a rigorous mathematical proof for this numerical scheme, it has been successfully applied to a variety of field problems. The development of this technique for problems of flow through porous media has been presented by Garder, Peaceman, and Pozzi (1964), Pinder and Cooper (1970), Reddell and Sunada (1970), and Bredehoeft and Pinder (1973). Garder, Peaceman, and Pozzi (1964) state that this technique does not introduce numerical dispersion (artificial dispersion resulting from the numerical calculation process). They and Reddell and Sunada (1970) also compared solutions obtained using the method of characteristics with those derived by analytical methods and found good agreement for the cases investigated. Applications of the method to field problems have been documented by Bredehoeft and Pinder (1973), Konikow and Bredehoeft (1974), Robertson (1974), Robson (1974), and Konikow (1977).

The approach taken by the method of characteristics is not to solve equation 4 directly, but rather to solve an equivalent system of ordinary differential equations. Konikow and Grove (1977, eq 61) show that by considering saturated thickness as a variable and by expanding the convective transport term, equation 4 may be rewritten as

$$\frac{\partial C}{\partial t}=\frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right)-V_i\frac{\partial C}{\partial x_i}+\frac{C\left(S\frac{\partial h}{\partial t}+W-\epsilon\frac{\partial b}{\partial t}\right)-C'W}{\epsilon b}. \quad (14)$$

Equation 14 is the form of the solute-transport equation that is solved in the computer program presented in this report. For convenience we may also write equation 14 as

$$\frac{\partial C}{\partial t}=\frac{1}{b}\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right)-V_x\frac{\partial C}{\partial x}-V_y\frac{\partial C}{\partial y}+F \quad (15)$$

where

$$F=\frac{C(S\frac{\partial h}{\partial t}+W-\epsilon\frac{\partial b}{\partial t})-C'W}{\epsilon b}. \quad (16)$$

Next consider representative fluid particles that are convected with flowing ground water. Note that changes with time in properties of the fluid, such as concentration, may be described either for fixed points within a stationary coordinate system as successive fluid particles pass the reference points, or for reference fluid particles as they move along their respective paths past fixed points in space. Aris (1962, p. 78) states that "associated with these two descriptions are two derivatives with respect to time." Thus $\partial C/\partial t$ is the rate of change of concentration as observed from a fixed point, whereas dC/dt is the rate of change as observed when moving with the fluid particle. Aris (1962) calls the latter the *material derivative.*

The material derivative of concentration may be defined as

$$\frac{dC}{dt}=\frac{\partial C}{\partial t}+\frac{\partial C}{\partial x}\frac{dx}{dt}+\frac{\partial C}{\partial y}\frac{dy}{dt}. \quad (17)$$

Note the correspondence of the second and third terms on the right side of equation 15 with the second and third terms on the right side of equation 17. The latter includes the material derivatives of position, which are defined by velocity. Thus for the x and y components, respectively, of position and velocity we have

$$\frac{dx}{dt}=V_x \quad (18)$$

and

$$\frac{dy}{dt}=V_y. \quad (19)$$

If we next substitute the right sides of equations 15, 18, and 19 for the corresponding terms in equation 17, we obtain

$$\frac{dC}{dt}=\frac{1}{b}\frac{\partial}{\partial x_i}(bD_{ij}\frac{\partial C}{\partial x_j})+F. \quad (20)$$

The solutions of the system of equations comprising equations 18–20 may be given as

$$x=x(t)\,;\ y=y(t)\,;\ \text{and}\ C=C(t) \quad (21)$$

and are called the characteristic curves of equation 15.

Given solutions to equations 18–20, a solution to the partial differential equation (eq 15) may be obtained by following the characteristic curves. This is accomplished numerically by introducing a set of moving points (or reference particles) that can be traced within the stationary coordinates of the finite-difference grid. Garder, Peaceman, and Pozzi (1964, p. 27) state, "Each point corresponds to one characteristic curve, and values of x, y, and C are obtained as functions of t for each characteristic." Each point has a concentration and position associated with it and is moved through the flow field in proportion to the flow velocity at its location. Intuitively, the method may be visualized as tracing a number of fluid particles through a flow field and observing changes in chemical concentration in the fluid particles as they move.

Particle tracking

The first step in the method of characteristics involves placing a number of traceable particles or points in each cell of the finite-difference grid to form a set of points that are distributed in a geometrically uniform pattern throughout the area of interest. It was found that placing from four to nine points per cell provided satisfactory results for most two-dimensional problems. The location or position of each particle is specified by its x- and y- coordinates in the finite-difference grid. The initial concentration assigned to each point is the initial concentration associated with the node of the cell containing the point.

For each time step every point is moved a distance proportional to the length of the time increment and the velocity at the location of the point. (See fig. 1.) The new position of a point is thus computed with the following finite-difference forms of equations 18 and 19:

$$x_{p,k}=x_{p,k-1}+\delta x_p=x_{p,k-1}+\Delta t V_{x[x_{(p,k)},y_{(p,k)}]} \quad (22)$$

and

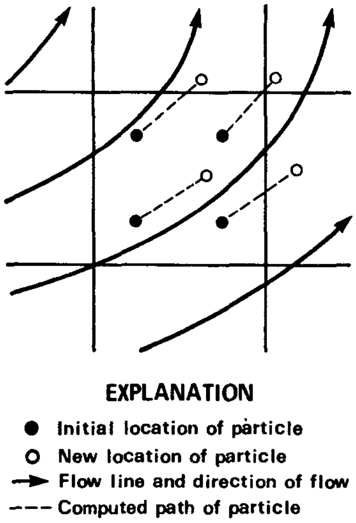


Figure 1.—Part of hypothetical finite-difference grid showing relation of flow field to movement of points.

$$y_{p,k}=y_{p,k-1}+\delta y_p=y_{p,k-1}+\Delta t V_{y[x_{(p,k)},y_{(p,k)}]} \qquad (23)$$

where

p is the index number for point identification; and

δx_p and δy_p are the distances moved in the x and y directions, respectively.

The x and y velocities at the position of any particular point p, indicated as $V_{i[x_{(p,k)},y_{(p,k)}]}$, for time k are calculated through bilinear interpolation over the area of half of a cell using the x and y velocities computed at adjacent nodes and cell boundaries. For example, figure 2 illustrates that the velocity in the x direction of point p, located in the southeast quadrant of cell (i,j), would be computed using bilinear interpolation between the x velocities computed with equations 12 and 13 at (i,j), $(i,j+1)$, $(i+1/2,j)$, and $(i+1/2,j+1)$. Similarly, the velocity in the y direction of point p would be based on the y velocities computed at (i,j), $(i+1,j)$, $(i,j+1/2)$ and $(i+1,j+1/2)$.

After all points have been moved, the concentration at each node is temporarily assigned the average of the concentrations of all points then located within the area of that cell; this average concentration is denoted as C_{i,j,k^*}. The time index is distinguished with an asterisk here because this temporarily assigned average concentration represents the new time level only with respect to convective transport. The moving points simulate convective transport because the concentration at each node of the grid will change with each time step as different points having different concentrations enter and leave the area of that cell.

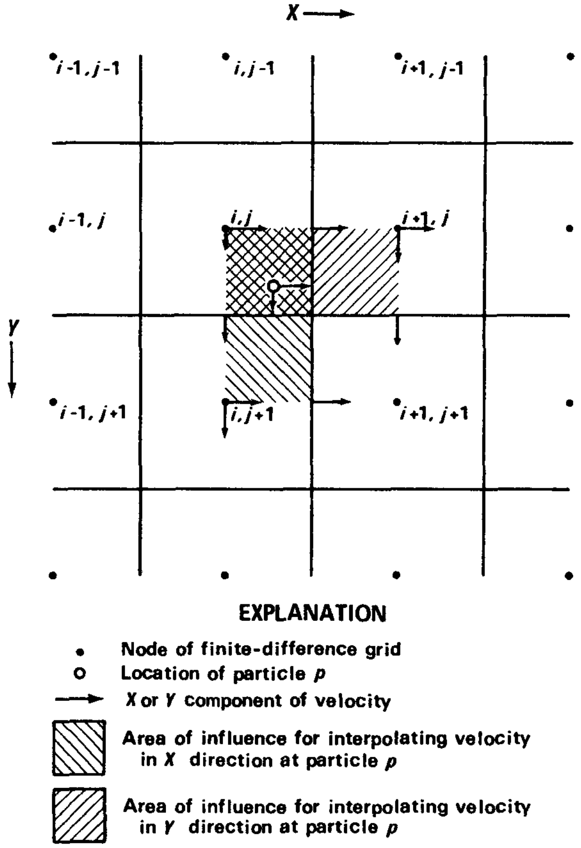


Figure 2.—Part of hypothetical finite-difference grid showing areas over which bilinear interpolation is used to compute the velocity at a point. Note that each area of influence is equal to one-half of the area of a cell.

Finite-difference approximations

The total change in concentration in an aquifer may be computed by solving equations 18–20. Equations 18 and 19, which are related to changes in concentration caused by convective transport alone, are solved by the movement of points as described previously. The changes in concentration caused by hydrodynamic dispersion, fluid sources, divergence of velocity, and changes in saturated thickness are calculated using an explicit finite-difference approximation to equation 20, which can be expressed as

$$\Delta C_{i,j,k}=\Delta t\left[\frac{1}{b}\frac{\partial}{\partial x_i}(bD_{ij}\frac{\partial C}{\partial x_j})+F\right]. \quad (24)$$

Note that a solution to equation 20 requires the computation of the change in concentration at the tracer particles. However, primarily because of the difficulty in computing the concentration gradient at a large number of moving points, the change in concentration represented by equation 20 is solved at each node of the grid rather than directly at the location of each point. The material derivative of concentration on any characteristic curve (or for any tracer particle) is then related to the change in concentration for a node during one time step, which was computed with the solution to equation 24.

The right side of equation 24 can be considered as the sum of two separate terms, as follows:

$$\Delta C_{i,j,k}=(\Delta C_{i,j,k})_{\mathrm{I}}+(\Delta C_{i,j,k})_{\mathrm{II}} \quad (25)$$

where

$(\Delta C_{i,j,k})_{\mathrm{I}}$ is the change in concentration caused by hydrodynamic dispersion, and is defined as

$$(\Delta C_{i,j,k})_{\mathrm{I}}=\frac{\Delta t}{b}[\frac{\partial}{\partial x_i}(bD_{ij}\frac{\partial C}{\partial x_j})] \quad (26)$$

and

$(\Delta C_{i,j,k})_{\mathrm{II}}$ is the change in concentration resulting from an external fluid source and changes in saturated thickness, and from equation 16 is defined as

$$(\Delta C_{i,j,k})_{\mathrm{II}}=\Delta t\,F$$

$$=\Delta t\left[\frac{C(S\frac{\partial h}{\partial t}+W-\epsilon\frac{\partial b}{\partial t})-C'W}{\epsilon b}\right]. \quad (27)$$

First we will examine the change in concentration due to dispersion, partly following the development of Reddell and Sunada (1970). The right side of equation 26 can be expanded according to the summation convention of tensor notation to obtain

$$(\Delta C_{i,j,k})_{\mathrm{I}}=\frac{\Delta t}{b}\left[\frac{\partial}{\partial x}(bD_{xx}\frac{\partial C}{\partial x}+bD_{xy}\frac{\partial C}{\partial y})+\frac{\partial}{\partial y}(bD_{yy}\frac{\partial C}{\partial y}+bD_{yx}\frac{\partial C}{\partial x})\right]. \quad (28)$$

A finite-difference approximation for the derivative in the x direction at (i,j) may be written as

$$\frac{\partial}{\partial x}(bD_{xx}\frac{\partial C}{\partial x}+bD_{xy}\frac{\partial C}{\partial y})$$

$$=\frac{\partial}{\partial x}(bD_{xx}\frac{\partial C}{\partial x})+\frac{\partial}{\partial x}(bD_{xy}\frac{\partial C}{\partial y})$$

$$=\frac{\left(bD_{xx}\frac{\partial C}{\partial x}\right)_{i+\frac{1}{2},j}-\left(bD_{xx}\frac{\partial C}{\partial x}\right)_{i-\frac{1}{2},j}}{\Delta x}+\frac{\left(bD_{xy}\frac{\partial C}{\partial y}\right)_{i+\frac{1}{2},j}-\left(bD_{xy}\frac{\partial C}{\partial y}\right)_{i-\frac{1}{2},j}}{\Delta x}. \quad (29)$$

In the following expansion of equation 29 it is implied that concentrations (C) are known from the previous (k–1) time level; hence, equation 29 is an explicit finite-difference equation. The spatial derivatives of concentration at $(i+\frac{1}{2},j)$ may be approximated by

$$\left(\frac{\partial C}{\partial x}\right)_{i+\frac{1}{2},j}=\frac{C_{i+1,j}-C_{i,j}}{\Delta x} \quad (30)$$

and

$$\left(\frac{\partial C}{\partial y}\right)_{i+\frac{1}{2},j}=\frac{C_{i+\frac{1}{2},j+1}-C_{i+\frac{1}{2},j-1}}{2\Delta y}. \quad (31)$$

Because concentrations are defined only at nodes, we must express the right side of equation 31 in terms of concentrations at nodes. Assuming that the concentration at a cell boundary is approximately equal to the average (arithmetic mean) of the concentrations at adjacent nodes, we have

$$C_{i+\frac{1}{2},j+1}=\frac{C_{i,j+1}+C_{i+1,j+1}}{2} \tag{32}$$

and

$$C_{i+\frac{1}{2},j-1}=\frac{C_{i,j-1}+C_{i+1,j-1}}{2}. \tag{33}$$

Substitution of equations 32 and 33 into equation 31 results in:

$$\left(\frac{\partial C}{\partial y}\right)_{i+\frac{1}{2},j}=\frac{C_{i,j+1}+C_{i+1,j+1}-C_{i,j-1}-C_{i+1,j-1}}{4\Delta y}. \tag{34}$$

Similarly, the spatial derivatives of concentration at $(i-\frac{1}{2},j)$ are

$$\left(\frac{\partial C}{\partial x}\right)_{i-\frac{1}{2},j}=\frac{C_{i,j}-C_{i-1}}{\Delta x} \tag{35}$$

and

$$\left(\frac{\partial C}{\partial y}\right)_{i-\frac{1}{2},j}=\frac{C_{i-1,j+1}+C_{i,j+1}-C_{i-1,j-1}-C_{i,j-1}}{4\Delta y}. \tag{36}$$

After substituting equations 30, 34, 35, and 36 into equation 29, we have

$$\begin{aligned}\frac{\partial}{\partial x}\left(bD_{xx}\frac{\partial C}{\partial x}+bD_{xy}\frac{\partial C}{\partial y}\right)
&=\frac{bD_{xx[i+\frac{1}{2},j]}(C_{i+1,j}-C_{i,j})}{(\Delta x)^2}-\frac{bD_{xx[i-\frac{1}{2},j]}(C_{i,j}-C_{i-1,j})}{(\Delta x)^2}\\
&+\frac{bD_{xy[i+\frac{1}{2},j]}(C_{i,j+1}+C_{i+1,j+1}-C_{i,j-1}-C_{i+1,j-1})}{4\Delta x\Delta y}\\
&-\frac{bD_{xy[i-\frac{1}{2},j]}(C_{i-1,j+1}+C_{i,j+1}-C_{i-1,j-1}-C_{i,j-1})}{4\Delta x\Delta y}.\end{aligned} \tag{37}$$

A finite-difference approximation for the derivative in the y direction in equation 28 may be developed for node (i,j) in an analogous manner to equation 37 to produce

$$\begin{aligned}\frac{\partial}{\partial y}\left(bD_{yy}\frac{\partial C}{\partial y}+bD_{yx}\frac{\partial C}{\partial x}\right)
&=\frac{\left(bD_{yy}\frac{\partial C}{\partial y}\right)_{i,j+\frac{1}{2}}-\left(bD_{yy}\frac{\partial C}{\partial y}\right)_{i,j-\frac{1}{2}}}{\Delta y}+\frac{\left(bD_{yx}\frac{\partial C}{\partial x}\right)_{i,j+\frac{1}{2}}-\left(bD_{yx}\frac{\partial C}{\partial x}\right)_{i,j-\frac{1}{2}}}{\Delta y}\\
&=\frac{bD_{yy[i,j+\frac{1}{2}]}(C_{i,j+1}-C_{i,j})}{(\Delta y)^2}-\frac{bD_{yy[i,j-\frac{1}{2}]}(C_{i,j}-C_{i,j-1})}{(\Delta y)^2}\\
&+\frac{bD_{yx[i,j+\frac{1}{2}]}(C_{i+1,j}+C_{i+1,j+1}-C_{i-1,j}-C_{i-1,j+1})}{4\Delta x\Delta y}\\
&-\frac{bD_{yx[i,j-\frac{1}{2}]}(C_{i+1,j-1}+C_{i+1,j}-C_{i-1,j-1}-C_{i-1,j})}{4\Delta x\Delta y}.\end{aligned} \tag{38}$$

Equation 28 may then be solved explicitly by substituting the relationships expressed by equations 37 and 38 for the terms within brackets on the right side of equation 28.

Next we will examine the change in concentration denoted by equation 27. Substituting explicit finite-difference approximations for the terms in equation 27, we have

$$(\Delta C_{i,j,k})_{II} = \frac{\Delta t}{\epsilon b_{i,j,k}}\Bigg[C_{i,j,k-1}\Bigg(S\left[\frac{h_{i,j,k}-h_{i,j,k-1}}{\Delta t}\right] + W_{i,j,k} - \epsilon\left[\frac{b_{i,j,k}-b_{i,j,k-1}}{\Delta t}\right]\Bigg) - C'_{i,j,k}W_{i,j,k}\Bigg]. \quad (39)$$

Equations 28, 37, 38, and 39 together provide a solution to equation 24, which in turn allows us to solve equation 20 and complete the definition of the characteristic curves of equation 15.

Because the processes of convective transport, hydrodynamic dispersion, and mixing are occurring continuously and simultaneously, equations 18, 19, and 20 should be solved simultaneously. However, equations 18 and 19 are solved by particle movement based on implicitly computed heads while equation 20 is solved explicitly with respect to concentrations. Because the change in concentration at a source node due to mixing is proportional to the difference in concentration between the node and the source fluid (see eq 27), the accuracy of estimating the concentration at the node during a time increment will clearly affect the computed change. Similarly, because the change in concentration due to dispersion is proportional to the concentration gradient at a point, the accuracy of estimating the concentration gradient will clearly affect the accuracy of the numerical results. As the position of a front or breakthrough curve advances with time, say from the $k-1$ to k time level, the concentration gradient at any fixed reference point and the concentration differences at sources are continuosly changing. The consequent limitations imposed by estimating nodal concentrations in a strict explicit manner can be minimized by using a two-step explicit procedure in which equation 24 is solved at each node by giving equal weight to concentration gradients computed from the concentrations at the previous time level $(k-1)$ and to concentration gradients computed from concentrations at time level (k^*), which represents the convected position of the front at the new time level (k) prior to adjustments of concentration for dispersion and mixing. Figure 3 illustrates the sequence of calculations to solve equations 18–20 over a given time increment. First the concentration gradients at the previous time level $(k-1)$ are determined at each node. Then the front is convected to a new position for time level k^* based on the velocity of flow and length of the time increment. Next the concentration gradients at each node are recomputed for the new position of the front. The concentration distribution for the new frontal position is then adjusted at each node in two steps: first based on concentration gradients at $k-1$ and second based on concentration gradients at k^*.

The finite-difference approximation to equation 24 may thus be expressed as

$$\Delta C_{i,j,k} = \frac{0.5\,\Delta t}{b}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C_{(k-1)}}{\partial x_j}\right) + \frac{C_{(k-1)}\left(S\frac{\partial h}{\partial t} + W - \epsilon\frac{\partial b}{\partial t}\right) - C'W}{\epsilon}\right] + \frac{0.5\,\Delta t}{b}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C_{(k^*)}}{\partial x_j}\right) + \frac{C_{(k^*)}\left(S\frac{\partial h}{\partial t} + W - \epsilon\frac{\partial b}{\partial t}\right) - C'W}{\epsilon}\right] \quad (40)$$

in which the appropriate finite-difference approximations for the terms within brackets are indicated by equations 37, 38, and 39.

The new nodal concentrations at the end of time increment k are computed as

$$C_{i,j,k} = C_{i,j,k^*} + \Delta C_{i,j,k} \quad (41)$$

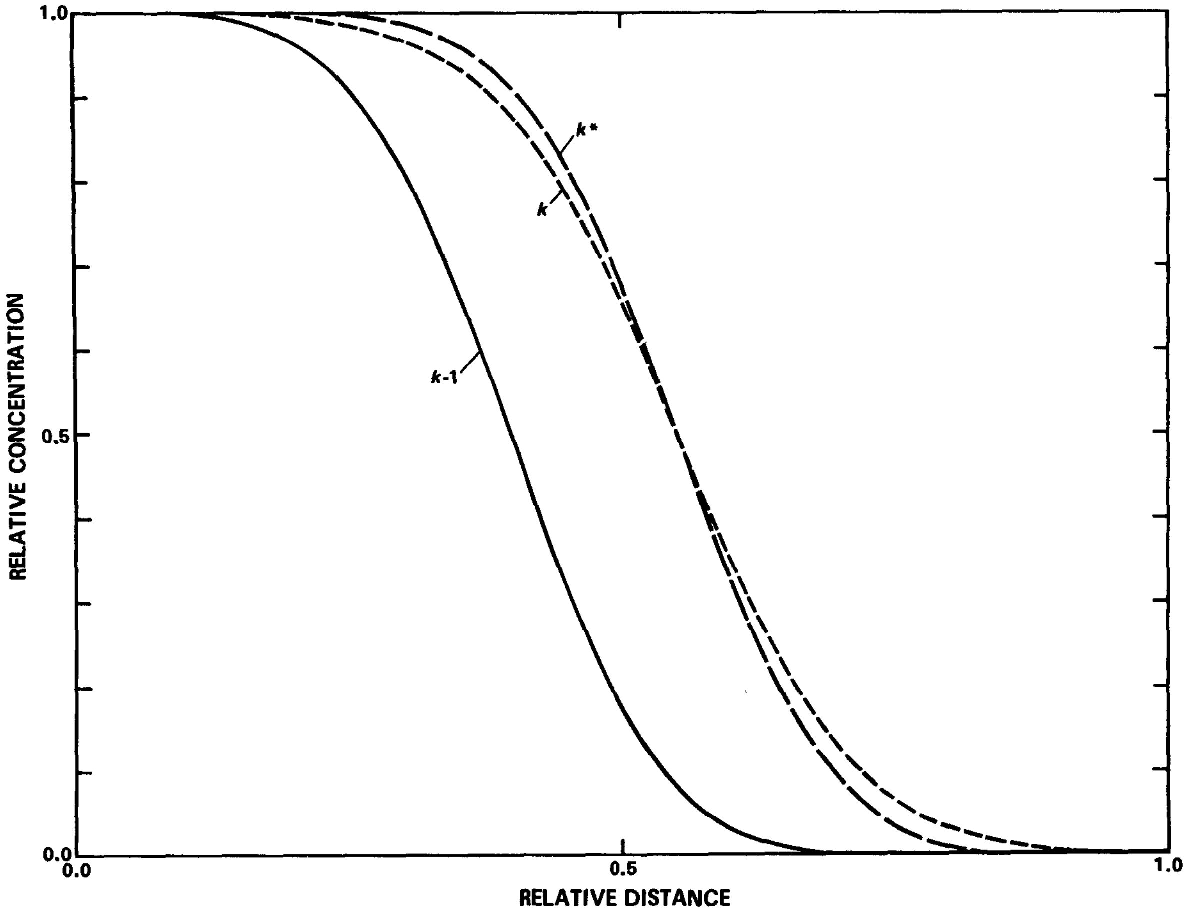


Figure 3.—Representative change in breakthrough curve from time level $k-1$ to k. Note that concentration changes are exaggerated to help illustrate the sequence of calculations.

where $C_{i,j,k*}$ is the average of the concentrations of all points in cell (i,j) after equations 22 and 23 were solved for all points for time step k, and $\Delta C_{i,j,k}$ is the change in concentration caused by hydrodynamic dispersion, sources, and sinks, as calculated in equation 40.

Because the concentrations of points in a cell vary about the concentration of the node, the change in concentration computed at a node using equation 40 cannot be applied directly in all cases to the concentrations of the points. If the change in concentration at the node ($\Delta C_{i,j,k}$) is positive, the increase is simply added to the point concentrations. But if the concentration change is negative, it is applied to points in that cell as a percentage decrease in concentration at each point that is equal to the percentage decrease at the node. This technique preserves a mass balance within each cell, but when a decrease in concentration is computed for a node, it will also prevent a possible but erroneous computation of negative concentrations at those points that had a concentration less than that at the node.

Stability criteria

The explicit numerical solution of the solute-transport equation has a number of stability criteria associated with it. These may require that the time step used to solve the flow equation be subdivided into a number of smaller time increments to accurately solve the solute-transport equation.

First, Reddell and Sunada (1970, p. 62) show that for an explicit finite-difference solution of equation 26 to be stable,

$$\frac{D_{xx}\,\Delta t}{(\Delta x)^2}+\frac{D_{yy}\,\Delta t}{(\Delta y)^2}\leq\frac{1}{2}. \qquad (42)$$

Solving equation 42 for Δt, we see that

$$\Delta t\leq \underset{\text{(over grid)}}{\text{Min}}\left[\frac{0.5}{\dfrac{D_{xx}}{(\Delta x)^2}+\dfrac{D_{yy}}{(\Delta y)^2}}\right]. \qquad (43)$$

Because the solution to equation 26 is actually written as a set of N equations for N nodes, the maximum permissible time increment is the smallest Δt computed for any individual node in the entire grid. The smallest Δt will then occur at the node having the largest value of

$$\frac{D_{xx}}{(\Delta x)^2}+\frac{D_{yy}}{(\Delta y)^2}.$$

Next consider the effects of mixing ground water of one concentration with injected or recharged water of a different concentration, as represented by the source terms in equation 39. The change in concentration in a source node cannot exceed the difference between the source concentration ($C'_{i,j}$) and the concentration in the aquifer ($C_{i,j}$), and the maximum possible change occurs when a source completely flushes out the volume of water in an aquifer cell at the start of a time step. Therefore

$$\Delta C_{i,j,k}\leq C_{i,j,k-1}-C'_{i,j,k}\,. \qquad (44)$$

After rearranging terms in equation 44, we have

$$\frac{\Delta C_{i,j,k}}{(C_{i,j,k-1}-C'_{i,j,k})}\leq 1.0. \qquad (45)$$

We may isolate the effects of mixing represented in equation 39 by assuming steady-state flow in which $\partial h/\partial t=0$ and $\partial b/\partial t=0$. Then we can rewrite equation 39 as

$$(\Delta C_{i,j,k})_{\text{II}}=\frac{\Delta t\,W_{i,j,k}\,(C_{i,j,k-1}-C'_{i,j,k})}{\epsilon b_{i,j,k}}. \qquad (46)$$

After rearranging terms in equation 46, we have

$$\frac{(\Delta C_{i,j,k})_{\text{II}}}{(C_{i,j,k-1}-C'_{i,j,k})}=\frac{\Delta t\,W_{i,j,k}}{\epsilon b_{i,j,k}}. \qquad (47)$$

Substituting equation 47 into equation 45 results in

$$\frac{\Delta t\,W_{i,j,k}}{\epsilon b_{i,j,k}}\leq 1.0. \qquad (48)$$

Solving equation 48 for Δt at all nodes yields the following criterion:

$$\Delta t\leq \underset{\text{(over grid)}}{\text{Min}}\left[\frac{\epsilon b_{i,j,k}}{W_{i,j,k}}\right]. \qquad (49)$$

A third type of stability check involves the movement of points computed by equations 22 and 23 to simulate convective transport. The distance a particle moves is defined as

$$\delta x=\Delta t\;V_{x[x_{(p,k)},y_{(p,k)}]} \qquad (50)$$

and

$$\delta y=\Delta t\;V_{y[x_{(p,k)},y_{(p,k)}]}\,. \qquad (51)$$

In effect, this constitutes a linear spatial extrapolation of the position of a particle from one time step to the next. Where streamlines are curvilinear, the extrapolated position of a particle will deviate from the streamline on which it was previously located. This deviation introduces an error into the numerical solution that is proportional to Δt. Thus, it is thought that an accurate computation of concentration changes caused by convective transport requires the maintenance of a relatively uniformly spaced field of marker particles that are moving along relatively smooth and continuous pathlines. Also, if δx is greater than Δx, or δy is greater than Δy, it might be possible for particles to move beyond the boundaries of the grid during one time increment. Thus, for a given velocity field and grid, some restriction must be placed on the size of the time increment to assure that neither δx nor δy exceed some critical distances, called δx^* and δy^*. Therefore

$$\delta x\leq\delta x^* \qquad (52)$$

and

$$\delta y\leq\delta y^*. \qquad (53)$$

These critical distances can be related to the dimensions of the finite-difference grid by

$$\delta x^*=\gamma\Delta x \qquad (54)$$

and

$$\delta y^* = \gamma \Delta y \qquad (55)$$

where γ is the fraction of the grid dimensions that particles will be allowed to move $(0 < \gamma \leq 1)$.

If we replace the terms in equations 52 and 53 with the corresponding terms from equations 50, 51, 54, and 55, we have

$$\Delta t \, V_{x[x_{(p,k)}, y_{(p,k)}]} \leq \gamma \Delta x \qquad (56)$$

and

$$\Delta t \, V_{y[x_{(p,k)}, y_{(p,k)}]} \leq \gamma \Delta y. \qquad (57)$$

Because these criteria are governed by the maximum velocities in the system, and since the computed velocity of a tracer particle will always be less than or equal to the maximum velocity computed at a node or cell boundary, we have to check only the latter. Substituting the grid velocities and solving equations 56 and 57 for Δt results in

$$\Delta t \leq \frac{\gamma \Delta x}{(V_x)_{\max}} \qquad (58)$$

and

$$\Delta t \leq \frac{\gamma \Delta y}{(V_y)_{\max}}. \qquad (59)$$

If the time step used to solve the flow equation exceeds the smallest of the time limits determined by equations 43, 49, 58, or 59, then the time step will be subdivided into the appropriate number of smaller time increments required for solving the solute-transport equation.

Boundary and initial conditions

Obtaining a solution to the equations that describe ground-water flow and solute transport requires the specification of boundary and initial conditions for the domain of the problem. Specifications for solving the flow equation must be compatible with the solution of the solute-transport equation. Several different types of boundary conditions can be incorporated into the solute-transport model. Two general types are incorporated in this model; these are constant-flux and constant-head conditions. These can be used to represent the real boundaries of an aquifer as well as to represent artificial boundaries for the model. The use of the latter can help to minimize data requirements and the areal extent of the modeled part of the aquifer.

A constant-flux boundary can be used to represent aquifer underflow, well withdrawals, or well injection. A finite flux is designated by specifying the flux rate as a well discharge or injection rate for the appropriate nodes. A no-flow boundary is a special case of a constant-flux boundary. The numerical procedure used in this model requires that the area of interest be surrounded by a no-flow boundary. Thus the model will automatically specify the outer rows and columns of the finite-difference grid as no-flow boundaries. No-flow boundaries can also be located elsewhere in the grid to simulate natural limits or barriers to ground-water flow. No-flow boundaries are designated by setting the transmissivity equal to zero at appropriate nodes, thereby precluding the flow of water or dissolved chemicals across the boundaries of the cell containing that node.

A constant-head boundary in the model can represent parts of the aquifer where the head will not change with time, such as recharge boundaries or areas beyond the influence of hydraulic stresses. In this model constant-head boundaries are simulated by adjusting the leakage term (the last term on the right side of equation 11) at the appropriate nodes. This is accomplished by setting the leakance coefficient (K_z/m) to a sufficiently high value (such as 1.0 s^{-1}) to allow the head in the aquifer at a node to be implicitly computed as a value that is essentially equal to the value of H_s, which in this case would be specified as the desired constant-head altitude. The resulting rate of leakage into or out of the designated constant-head cell would equal the flux required to maintain the head in the aquifer at the specified constant-head altitude.

If a constant-flux or constant-head boundary represents a fluid source, then the chemical concentration in the source fluid (C') must also be specified. If the boundary represents a fluid sink, then the concentration of the produced fluid will equal the concentration in the aquifer at the location of the sink.

Because solute transport directly depends upon hydraulic and concentration gradients, the head and concentration in the aquifer at the start of the simulation period must be specified. The initial conditions can be determined from field data and (or) from previous simulations. It is important to note that the simulation results may be sensitive to variations or errors in the initial conditions. In discussing computed heads, Trescott, Pinder, and Larson (1976, p. 30) state:

> If initial conditions are specified so that transient flow is occurring in the system at the start of the simulation, it should be recognized that water levels will change during the simulation, not only in response to the new pumping stress, but also due to the initial conditions. This may or may not be the intent of the user.

Mass balance

Mass balance calculations are performed after specified time increments to help check the numerical accuracy and precision of the solution. The principle of conservation of mass requires that the cumulative sums of mass inflows and outflows (or net flux) must equal the accumulation of mass (or change in mass stored). The difference between the net flux and the mass accumulation is the mass residual (R_m) and is one measure of the numerical accuracy of the solution. Although a small residual does not prove that the numerical solution is accurate, a large error in the mass balance is undesirable and may indicate the presence of a significant error in the numerical solution.

The model uses two methods to estimate the error in the mass balance. Both are based on the magnitude of the mass residual, R_m, which is computed from

$$R_m = \Delta M_s - M_f \tag{60}$$

where

ΔM_s is the change in mass stored in the aquifer, M; and

M_f is the net mass flux, M.

The two mass terms, ΔM_s and M_f, are evaluated using the following equations:

$$\Delta M_s = \sum_i \sum_j b_{i,j}\epsilon \Delta x \Delta y (C_{i,j,k} - C_{i,j,o}) \tag{61a}$$

where $C_{i,j,o}$ is the initial concentration at node (i,j), M/L^3; and

$$M_f = \sum_i \sum_j \sum_k W_{i,j,k} \Delta x \Delta y \Delta t_k \, C'_{i,j,k}. \tag{61b}$$

The percent error (E) in the mass balance is computed first by comparing the residual with the average of the net flux and net accumulation, as

$$E_1 = \frac{100.0\,(M_f - \Delta M_s)}{0.5\,(M_f + \Delta M_s)}. \tag{62}$$

This is a good measure of the accuracy of the numerical solution when the flux and the change in mass stored are relatively large. However, equation 62 does not account for the initial mass of solute in the aquifer. If total fluxes are very small compared to the initial mass of solute in the aquifer, then equation 62 might indicate a relatively large error when the numerical solution is actually quite accurate. Therefore, the error may also be computed a second way by comparing the residual with the initial mass of solute (M_0) present in the aquifer, as

$$E_2 = \frac{100.0\,(M_f - \Delta M_s)}{M_0}. \tag{63}$$

Equation 63 provides a good measure of the accuracy of the numerical solution when fluxes are zero or relatively small. But when M_0 is zero or very small in comparison to ΔM_s, then E_2 becomes meaningless. This problem can be overcome by correcting M_0 in the denominator of equation 63 for the net mass flux, resulting in

$$E_3 = \frac{100.0\,(M_f - \Delta M_s)}{M_o - M_f}. \tag{64}$$

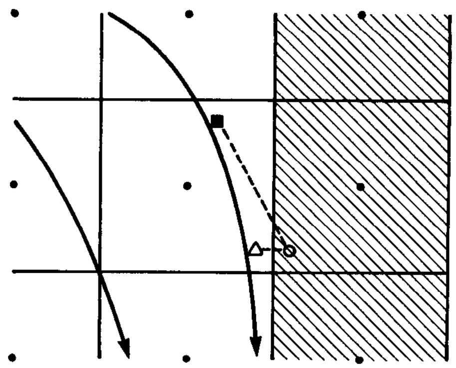
Note that as M_f becomes very small, equation 64 approaches equation 63, and as M_0 becomes very small, E_3 becomes just a comparison of the residual with the net flux. In the latter case E_3 is a mass balance indicator similar to E_1 in equation 62. Thus, E_3 is considered a more reliable and versatile indicator of numerical accuracy than is E_2. Either one or both of E_1 and E_3 are computed by the model, as appropriate.

Special problems

There are a number of special problems associated with the use of the method of characteristics to solve the solute-transport equation. Some of these problems are associated with the movement and tracking of particles, while other problems are related to the computational transition between the concentrations of particles within a cell and the average concentration at that node. We will next describe the more significant problems and the procedures used to minimize errors that might result from them.

One possible problem is related to no-flow boundaries. Neither water nor dissolved chemicals can be allowed to cross a no-flow boundary. However, under certain conditions it might be possible for the interpolated velocity at the location of a particle near a no-flow boundary to be such that the particle will be convected across the boundary during one time increment. Figure 4 illustrates such a possible situation, which arises from the deviation between the curvilinear flow line and the linearly projected particle path. If a particle is convected across a no-flow boundary, then it is relocated within the aquifer by reflection across the boundary, as also shown in figure 4. This correction thus will tend to relocate the particle closer to the true flow line.

Fluid sources and sinks also require special treatment. Because they tend to represent singularities in the velocity field, the use of a central difference formulation (eq 12) to compute the velocity at a node may indicate zero or very small velocities at the nodes. Therefore, the velocity components at a source or sink node cannot be used for interpolation of the velocity at a point within or adjacent to that cell. To help maintain radial flow to or from a sink or source, respectively, the velocities computed on the boundaries of source or sink cells are assigned to that node. The appropriate boundary velocities are determined on the basis of the quadrant of interest. This can be illustrated by referring again to figure 2. If a point is located in the southeast quadrant of cell (i,j), the x velocity at node (i,j) would



EXPLANATION

- • Node of finite-difference grid
- ■ Previous location of particle p
- o Computed new location of particle p
- Δ Corrected new location of particle p
- ⟶ Flow line and direction of flow
- --- Computed path of flow
- [hatched box] Zero transmissivity (or no-flow boundary)

Figure 4.—Possible movement of particles near an impermeable (no-flow) boundary.

be set equal to $V_{x(i+\frac{1}{2},j)}$ and the y velocity to $V_{y(i,j+\frac{1}{2})}$. Corresponding adjustments are made for points in other quadrants, so that the magnitude and direction of velocity at the node are not fixed for a given time increment, but depend on the relative location of the point of interest within the cell. A similar approximation is made when a point of interest is located in a cell adjacent to a source or sink. Thus, if the same point, p, in figure 2 were located in an unstressed cell but the adjacent cell $(i+1,j)$ represented a source or sink, then the y velocity at node $(i+1,j)$ would be approximated by $V_{y(i+1,j+\frac{1}{2})}$ in order to estimate the y velocity at point p. A corresponding approximation for the x velocity at node $(i,j+1)$ would be made using $V_{x(i+\frac{1}{2},j+1)}$ if a source or sink were located at $(i,j+1)$.

The maintenance of a reasonably uniform and continuous spacing of points requires special treatment in areas where sources and sinks dominate the flow field. Points will continually move out of a cell that represents a source, but few or none will move in to replace them and thereby maintain a continuous stream of points. Thus, whenever a point that originated in a source cell moves out of that source cell, a new point is introduced into the source cell to replace it. Placement of new points in a source cell is compatible with and analogous to the generation of fluid and solute mass at the source.

The procedure used to replace points in source cells that are adjacent to no-flow boundaries is illustrated in figure 5. Here a steady, uniformly spaced stream of points is maintained by generating a new point at the same relative position in the source cell as the new position in the adjacent cell of the point that left the source cell. As an example, point 7 was convected from cell $(i-1,j)$ to cell (i,j). So the replacement point (22) was placed at a location within cell $(i-1,j)$ that is identical to the new location of point 7 within cell (i,j).

The procedure used to replace points in source cells that lie within the aquifer and not adjacent to a no-flow boundary is illustrated in figure 6. Here a steady, uniformly spaced stream of particles is maintained by generating a new point in the source cell at the original location of the point that left the source cell. When a relatively strong source is imposed on a relatively weak regional flow field, as illustrated in figure 6a, then radial flow will be maintained in the area of the source, and all initial and replacement points will move symmetrically away from node (i,j). For example, after point 7 moves from cell (i,j) to $(i+1, j-1)$, the replacement point (18) is positioned at time k in cell (i,j) at the same location as the initial position of point 7. Although the replacement procedure illustrated earlier by figure 5 would work just as well for the case illustrated in figure 6a, it would not be satisfactory for the situation presented in figure 6b, which illustrates the imposition of a relatively weak source in a relatively strong regional flow field. In this case the velocity distribution within the source cell does not possess radial symmetry, and the velocity within the upgradient part of the source cell is much lower than the velocity within the downgradient part of the source cell. Replacement of points at original locations in source cells, as illustrated in figure 6b, will maintain a steady stream of points leaving the source cell in proportion to the velocity field. However, the use of the procedure illustrated in figure 5 for the case presented in figure 6b would result in the accumulation of

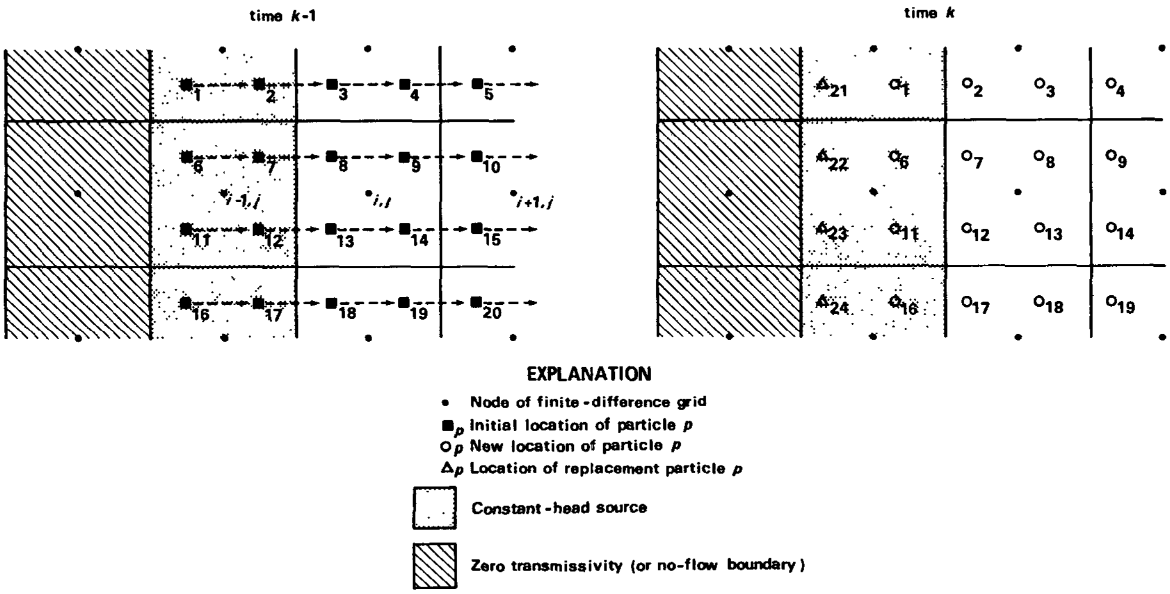


Figure 5.—Replacement of points in source cells adjacent to a no-flow boundary.

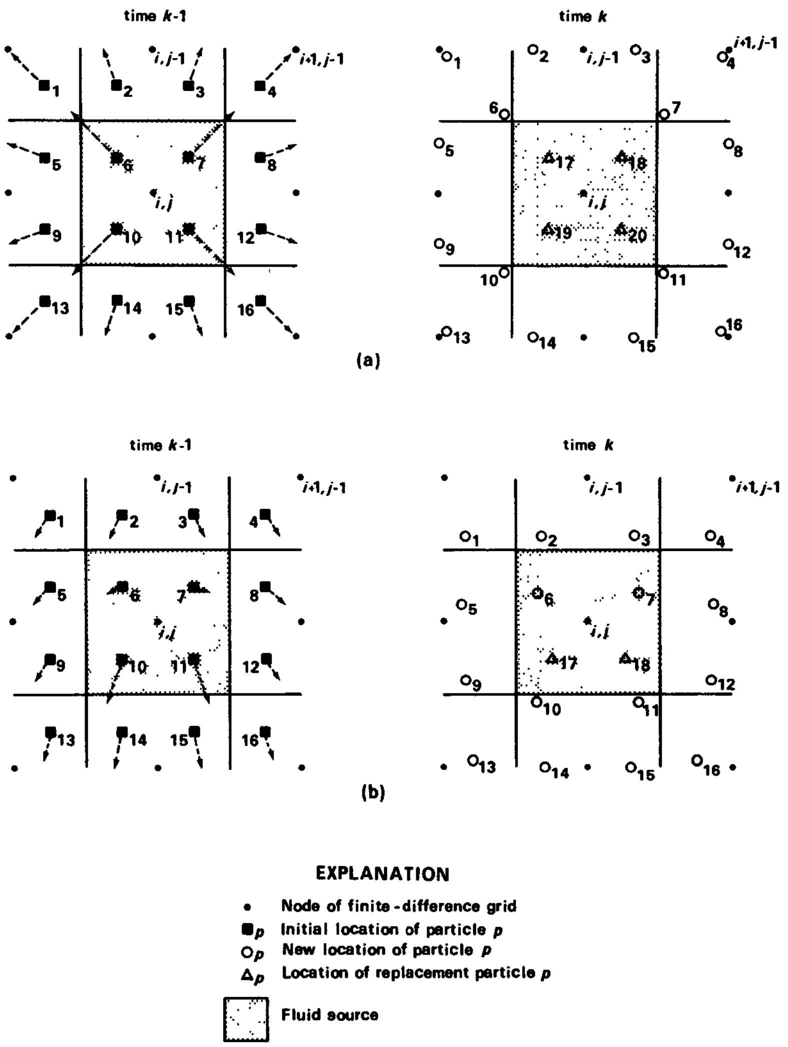


Figure 6.—Replacement of points in source cells not adjacent to a no-flow boundary for negligible regional flow (a) and for relatively strong regional flow (b).

points in the low-velocity area of the source cell (i,j), with few points being replaced into the high-velocity area, where convective transport is the greatest.

Although we normally expect points to be convected out of source cells, figure 6b also demonstrates the possibility that points may sometimes enter a source cell. This can also occur when two or more source cells of different strengths are adjacent to each other. An erroneous multiplication of points might then result if points that did not originate in a particular source cell are replaced when they in turn are convected out of that source cell. Therefore, points leaving a source cell are replaced only if they had originated in that source cell.

Hydraulic sinks also require some special treatment. Points will continually move into a cell representing a strong sink, but few or none will move out. To avoid the resultant crowding and stagnation of tracer points, any point moving into a sink cell is removed from the flow field after the calculations for that time increment have been completed. The numerical removal of points which enter sink cells is analogous to the withdrawal of fluid and solute mass through the hydraulic sink. The combination of creating new points at sources and destroying old points at sinks will tend to maintain the total number of points in the flow field at a nearly constant value.

Both the flow model and the transport model assume that sources and sinks act over the entire cell area surrounding a source or sink node. Thus, in effect, heads and concentrations computed at source or sink nodes represent average values over the area of the cell. Part of the total concentration change computed at a source node represents mixing between the source water at one concentration and the ground water at a different concentration (eq 39). It can be shown from the relationship between the source concentration ($C'_{i,j,k}$) and the aquifer concentration ($C_{i,j,k-1}$), as indicated by equation 44, that the following constraints generally must be met in a source cell:

$$C_{i,j,k} \leqq C'_{i,j,k} \quad \text{for} \quad C'_{i,j,k} > C_{i,j,k-1} \qquad \text{(65a)}$$

and

$$C_{i,j,k} \geqq C'_{i,j,k} \quad \text{for} \quad C'_{i,j,k} < C_{i,j,k-1}. \qquad \text{(65b)}$$

If it is assumed that the sources act over the area of the source cell and that there is complete vertical mixing, then these same constraints should also apply to all points within the cell. Because of the possible deviation of the concentrations of individual points within a source cell from the average concentration, the change in concentration computed at a source node ($\Delta C_{i,j,k}$) should not be applied directly to each of the points in the cell. Rather, at the end of each time increment the concentration of each point in a source cell is updated by setting it equal to the final nodal concentration. Although this may introduce a small amount of numerical dispersion by eliminating possible concentration variations within the area of a source cell, it prevents the adjustment of the concentration at any point in the source cell to a value that would violate the constraints indicated by equation 65.

In areas of divergent flow there may be a problem because some cells can become void of points where pathlines become spaced widely apart. This would result in a calculation of zero change in concentration at a node due to convective transport, although the nodal concentration would still be adjusted for changes caused by hydrodynamic dispersion (eq 28). Also, some numerical dispersion is generated at nodes in and adjacent to the cells into which the convective transport of solute was underestimated because of the resulting error in the concentration gradient. This might not cause a serious problem if only a few cells in a large grid became void or if the voiding were transitory (that is, if upgradient points were convected into void cells during later or subsequent time increments). Figure 6a illustrates radial flow, which represents the most severe case of divergent flow. Here it can be seen that when four points per cell are used to simulate convective transport, then in the numerical procedure four of the eight surrounding cells would erroneously not receive any solute by convection from the adjacent source. If eight points per cell were used initially, then at a distance of two rows or columns from the source only 8 of 16 cells would be on pathlines originating in the source cell. So, while increasing the initial number of points per cell would help, it is obvious that for purely radial flow, an impractically large initial number of points per cell would be required to be certain that at least one particle pathline passes from the source through every cell in the grid.

The problem of cells becoming void of particles can be minimized by limiting the number of void cells to a small percentage of the total number of cells that represent the aquifer. If the limit is exceeded, the numerical solution to the solute-transport equation is terminated at the end of that time increment and the "final" concentrations at that time are saved. Next the problem is reinitialized at the time of termination by regenerating the initial particle distribution throughout the grid and assigning the "final" concentrations at the time of termination as new "initial" concentrations for nodes and particles. The solution to the solute-transport equation is then simply continued in time from this new set of "initial" conditions until the total simulation period has elapsed. This procedure preserves the mass balance within each cell but also introduces a small amount of numerical dispersion by eliminating variations in concentration within individual cells.

To help minimize the amount of numerical dispersion resulting from the regeneration of points, the program also includes an optimization routine that attempts to maintain an approximation of the previous concentration gradient within a cell. The optimization routine aims to meet the following constraints:

$$\frac{\sum_{n=1}^{N_p} C_n^*}{N_p} = C_{i,j} \quad \text{(66a)}$$

$$C_{i,j} \leq C_n^* \leq C_{l,m} \quad \text{for} \quad C_{i,j} \leq C_{l,m} \quad \text{(66b)}$$

and

$$C_{l,m} \leq C_n^* \leq C_{i,j} \quad \text{for} \quad C_{i,j} \geq C_{l,m} \quad \text{(66c)}$$

where

C_n^* is the concentration of the nth point in cell (i,j), M/L^3;

N_p is the total number of points initially placed in a cell; and

$C_{l,m}$ is the concentration at node (l,m), which represents a cell adjacent to (i,j) and on a line that starts at (i,j) and extends through the coordinates of the point (n) of interest, as illustrated in figure 7, M/L^3.

Note that equation 66a simply indicates that a mass balance must be preserved in a cell regardless of the range in variation of point concentrations within the cell. Equations 66b and c indicate that the concentration of any point must lie between $C_{i,j}$ and the concentration at the node adjacent to particle n. The coordinates of the adjacent node would take on values of $l=i$ or $l=i\pm1$ and $m=j$ or $m=j\pm1$. For example, figure 7 shows that for point 2, the coordinates (l,m) would equal $(i,j-1)$, while for point 3, (l,m) would equal $(i+1,j-1)$. The optimization routine is written so that if equations 66a–c cannot be satisfied simultaneously for node (i,j) within two iterations, then to avoid further computational delay all C_n^* are simply set equal to $C_{i,j}$.

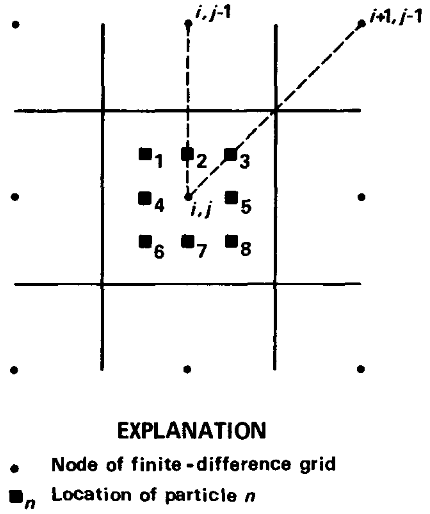


Figure 7.—Relation between possible initial locations of points and indices of adjacent nodes.

Computer Program

The computer program serves as a means of translating the numerical algorithm into machine executable instructions. The purpose of this chapter is to describe the overall structure of the program and to present a detailed description of its key elements, thereby providing a link between the numerical methods and the computer code. We hope that this link will make it easier for the model user to understand and, if necessary, modify the program. The FORTRAN IV source program developed for this model is listed in attachment I and includes almost 2,000 lines. For reference purposes columns 73–80 of each line contain a label that is numbered sequentially within each subroutine. The definition of selected variables used in the program is presented in attachment II; this glossary therefore also serves as a key for relating the program variables to their corresponding mathematical terms. The computer program is compatible with many scientific computers; it has been successfully run on Honeywell, IBM, DEC, and CDC computers.

General program features

The program is segmented into a main routine and eight subroutines. The name and primary purpose of each segment are listed in Table 1. Each program segment will be described in more detail in later sections of this chapter.

Table 1.—List of subroutines for solute-transport model

Name	Purpose
MAIN	Control execution.
PARLOD	Data input and initialization.
ITERAT	Compute head distribution.
GENPT	Generate or reposition particles.
VELO	Compute hydraulic gradients, velocities, dispersion equation coefficients, and time increment for stable solution to transport equation.
MOVE	Move particles.
CNCON	Compute change in chemical concentrations and compute mass balance for transport model.
OUTPT	Print head distribution and compute mass balance for flow model.
CHMOT	Print concentrations, chemical mass balance, and observation well data.

The major steps in the calculation procedures are summarized in figure 8, which presents a simplified flow chart of the overall structure of the computer program. The flow chart illustrates that the tracer particles may have to be moved more than once to complete a given time step. In other words, the time step used to implicitly solve the flow equation may have to be subdivided into a number of smaller time increments for the explicit solution of the solute-transport equation. The maximum time increments allowable for the explicit calculations are computed automatically by the model. Thus, the model user cannot specify an erroneously large increment or an inefficiently small increment for solving the solute-transport equation. For transient flow problems, some discretion is still required in the specification of the initial time step and of the time-step multiplier, as discussed by Trescott, Pinder, and Larson (1976, p. 38–40).

The general program presented here is written to allow a grid having up to 20 rows and 20 columns. Because the numerical procedure requires that the outer rows and columns represent no-flow boundaries, the aquifer itself is then limited to maximum dimensions of 18 rows and 18 columns. If a problem requires a larger grid, then the appropriate arrays must be redimensioned accordingly. These arrays are contained in COMMON statements PRMK, HEDA, HEDB, CHMA, CHMC, and DIFUS, and in DIMENSION statements on lines C170, G200, H140, and I160.

The program allows the specification of one pumping well per node. The wells can represent injection (recharge) or withdrawal (discharge). If more than one well exists within the area of a cell, then the flux specified for that node should represent the net rate of injection or withdrawal of all wells in that cell. The model assumes that stresses are constant with time during each pumping period (NPMP). But the total number of wells, as well as their locations, flux rates, and source concentrations, may be changed for successive pumping periods. The program also allows the specification of observation wells at as many as five nodes in the grid. For nodes that are designated as observation wells, at the end of the simulation period or after every 50 time increments the model will print a summary table of the head and concentration at the previous time increments.

The program also includes a node identification array (NODEID), which allows certain nodes or zones to be identified by a unique code number. This feature can save much time in the preparation of input data by easily equating each code number with a desired boundary condition, flux, or source concentration.

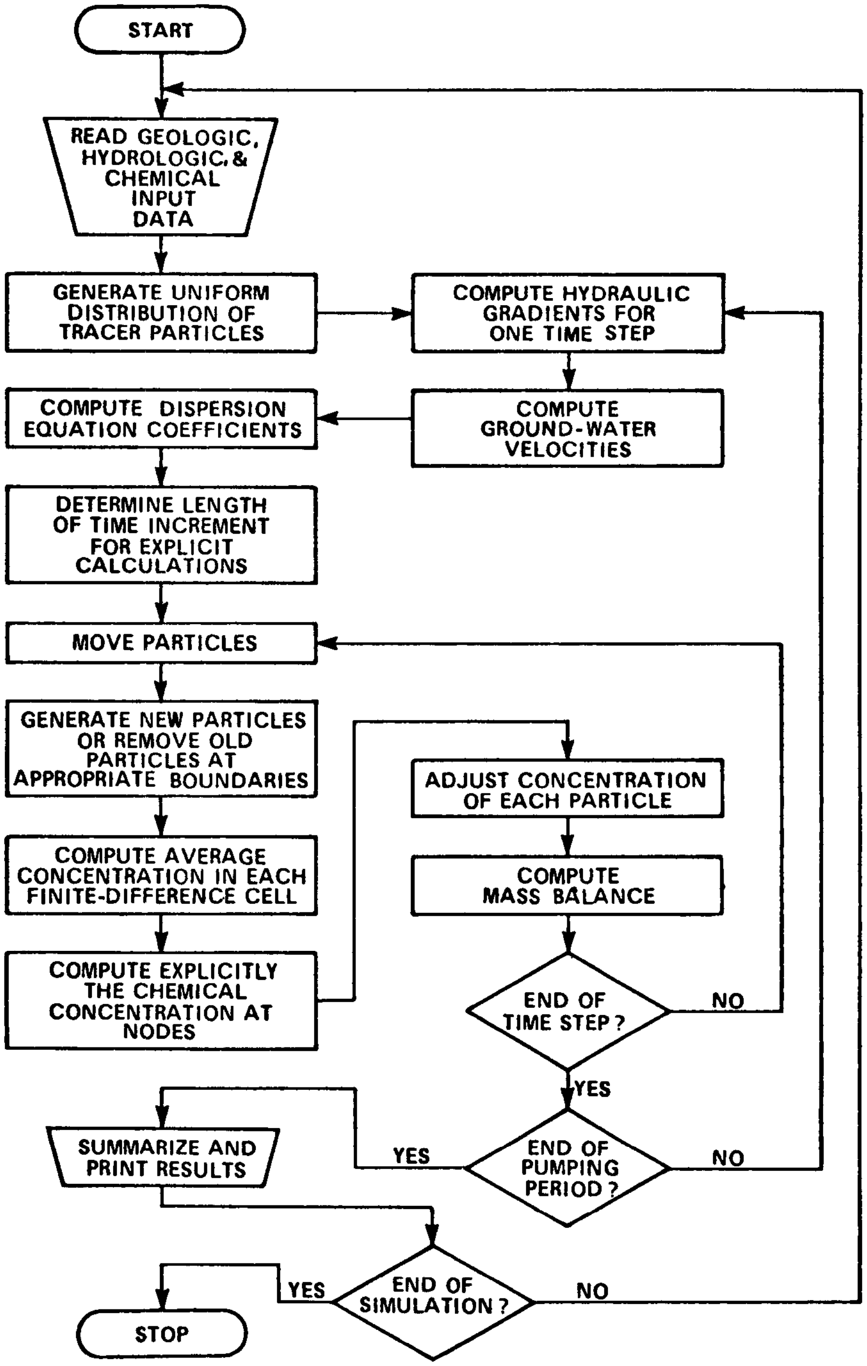


Figure 8.—Simplified flow chart illustrating the major steps in the calculation procedure.

Program segments

MAIN

The primary purpose of the MAIN routine is to control the overall execution sequence of the program. Subroutines for input, execution, and output are called from MAIN and the elapsed time simulated is compared with the desired total simulation period. Also, lines A500–A580 serve to store (or record) observation well data for transient flow problems.

Subroutine PARLOD

All input data are read through subroutine PARLOD. These data define the properties, boundaries, initial conditions, and stresses for the aquifer, as well as spatial grid and time-step factors. The values of many variables are also initialized here. After the data are read, some preliminary calculations are made, such as (1) determining time increments for the flow model (lines B780–B890), (2) computing the harmonic mean transmissivities in the x and y directions (B1670–B1800), (3) adjusting transmissivity for anisotropy (B1810–B1820), (4) computing iteration parameters (B1840–B1910 and B2880–B2980), and (5) checking for possible inconsistencies among the input data (B3140–B3290). A printout is also provided of all input data so that the data may be rechecked and each run identified.

Subroutine ITERAT

This subroutine solves a finite-difference approximation of the flow equation (eq 11) using an iterative ADI procedure. The matrix generated by the finite-difference approximation is solved using the Thomas algorithm, as described by von Rosenberg (1964, p. 113). Row calculations are made in lines C270–C610, and column calculations are made in lines C630–C970. The calculations are assumed to have converged on a solution if the maximum difference at all nodes between heads computed along rows and heads computed along columns is less than the specified tolerance. Convergence is checked on lines C940–C950. Note that here (for example, lines C380, C700, C930, and C1150) and in other subroutines the thickness array (THCK) is used to check whether a node is in the aquifer.

It should also be noted here that the flow model, as written, assumes that the transmissivity of the aquifer is independent of the head (or saturated thickness) and remains constant with time. If this assumption is not appropriate to the particular aquifer system being modeled, then the solution algorithm presented in this subroutine should be modified accordingly. For example, flow models published by Prickett and Lonnquist (1971, p. 43–45) and Trescott, Pinder, and Larson (1976) include such a modification.

All parameters involved in the calculation of heads are defined as double precision variables and all calculations involving these parameters are performed in double precision. The number of double precision variables and operations can be reduced significantly if the program is to be executed on a high-precision scientific computer, thereby improving the efficiency of the model by reducing computer storage requirements and execution time.

The iterative ADI procedure used to solve the finite-difference equations is not necessarily the best possible solution technique for all problems. For example, it may be difficult to obtain a solution using the iterative ADI procedure for cases of steady-state flow when internal nodes in the grid have zero transmissivity and for cases in which the transmissivity is highly anisotropic. In such cases, a strongly implicit procedure, such as the one documented by Trescott, Pinder, and Larson (1976), should be substituted for the solution algorithm contained in subroutine ITERAT.

Subroutine GENPT

The primary purpose of subroutine GENPT is to generate a uniform initial distribution of tracer particles throughout the finite-difference grid. This is done either at the start of a simulation period or at an intermediate time when too many cells have become void of particles. In the latter case, the program attempts to preserve an approximation of the previous concentration gradient within each cell (lines D1420–D2040).

The placement of particles is accomplished in lines D510–D1410. The program allows the placement of either four, five, eight, or nine particles per cell. Of course each option will result in a slightly different geometry

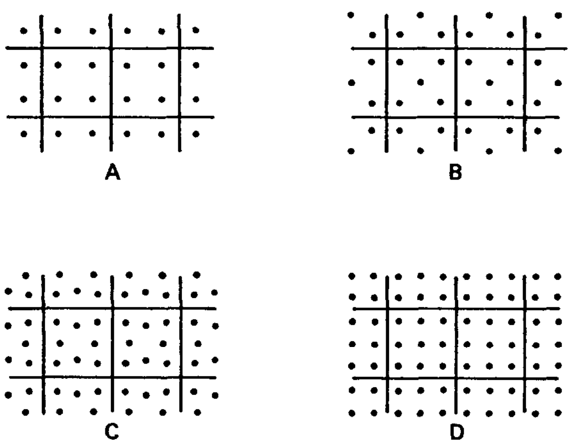


Figure 9.—Parts of finite-difference grids showing the initial geometry of particle distribution for the specification of four (*A*), five (*B*), eight (*C*), and nine (*D*) particles per cell.

and density of points, as illustrated by figure 9. The most regular or uniform patterns are produced when four or nine particles per cell are specified. If a different number of particles per cell or a different placement geometry are desired, this subroutine could be modified accordingly.

As particles are moved or convected through the grid during the calculation procedure, there is a need to remove particles at fluid sinks and create particles at fluid sources. A buffer array (called LIMBO) is created on lines D430–D480 that contains particles that can be added later to the grid at sources and that also contains space to store particles removed at sinks or discharge boundaries.

Subroutine VELO

Subroutine VELO accomplishes three objectives. First, it computes the flow velocities at nodes and on cell boundaries by solving equations having the form of equations 12 and 13. The velocities are computed on lines E420–E680. Second, the dispersion equation coefficients are calculated. These coefficients represent terms factored out of equations 37 and 38, as follows:

$$\text{DISP(IX,IY,1)} = (bD_{xx})_{[i+\frac{1}{2},j]}/(\Delta x)^2 \quad (67a)$$

$$\text{DISP(IX,IY,2)} = (bD_{yy})_{[i,j+\frac{1}{2}]}/(\Delta y)^2 \quad (67b)$$

$$\text{DISP(IX,IY,3)} = (bD_{xy})_{[i+\frac{1}{2},j]}/4\Delta x\Delta y \quad (67c)$$

$$\text{DISP(IX,IY,4)} = (bD_{yx})_{[i,j+\frac{1}{2}]}/4\Delta x\Delta y. \quad (67d)$$

Note that each dispersion coefficient (D_{xx}, D_{yy}, D_{xy}, D_{yx}) is computed on cell boundaries using the relationships expressed in equations 8–10. Therefore, the equation coefficients computed by equation 67 are stored as forward values from the indicated node in the DISP array. Third, this subroutine computes (on lines E1050–E1240 and E1800–E1930) the minimum number of particle moves (NMOV) required to solve the transport equation for the given time step so that the maximum time increment for the transport equation solution will not exceed any of the criteria indicated by equations 43, 49, 58, and 59.

Subroutine MOVE

Although this subroutine has only one main function, which is to move the tracer particles in accordance with equations 22 and 23, it is the longest and perhaps the most complex segment of the program. The complexities are mainly introduced by the treatment of particles at the various types of boundary conditions. To help illustrate the calculation procedure followed within subroutine MOVE, a flow chart is presented in figure 10. The numbers in the flow chart indicate the corresponding lines in subroutine MOVE where the indicated operation is executed.

If a node represents a fluid source or sink, then particles must be respectively created or destroyed in these cells. If the value of pumpage (REC) at a node does not equal zero, then the node is assumed to represent either a fluid source (for REC<0) or a fluid sink (for REC>0). Recharge or discharge can also be represented by the RECH array. But it is assumed that this type of flux is sufficiently diffuse so that it does not induce areas or points of strongly divergent or convergent flow and therefore particles need not be created or destroyed at these nodes. Note that here and in other subroutines the presence of a constant-head boundary is tested by checking the value of leakance (VPRM)

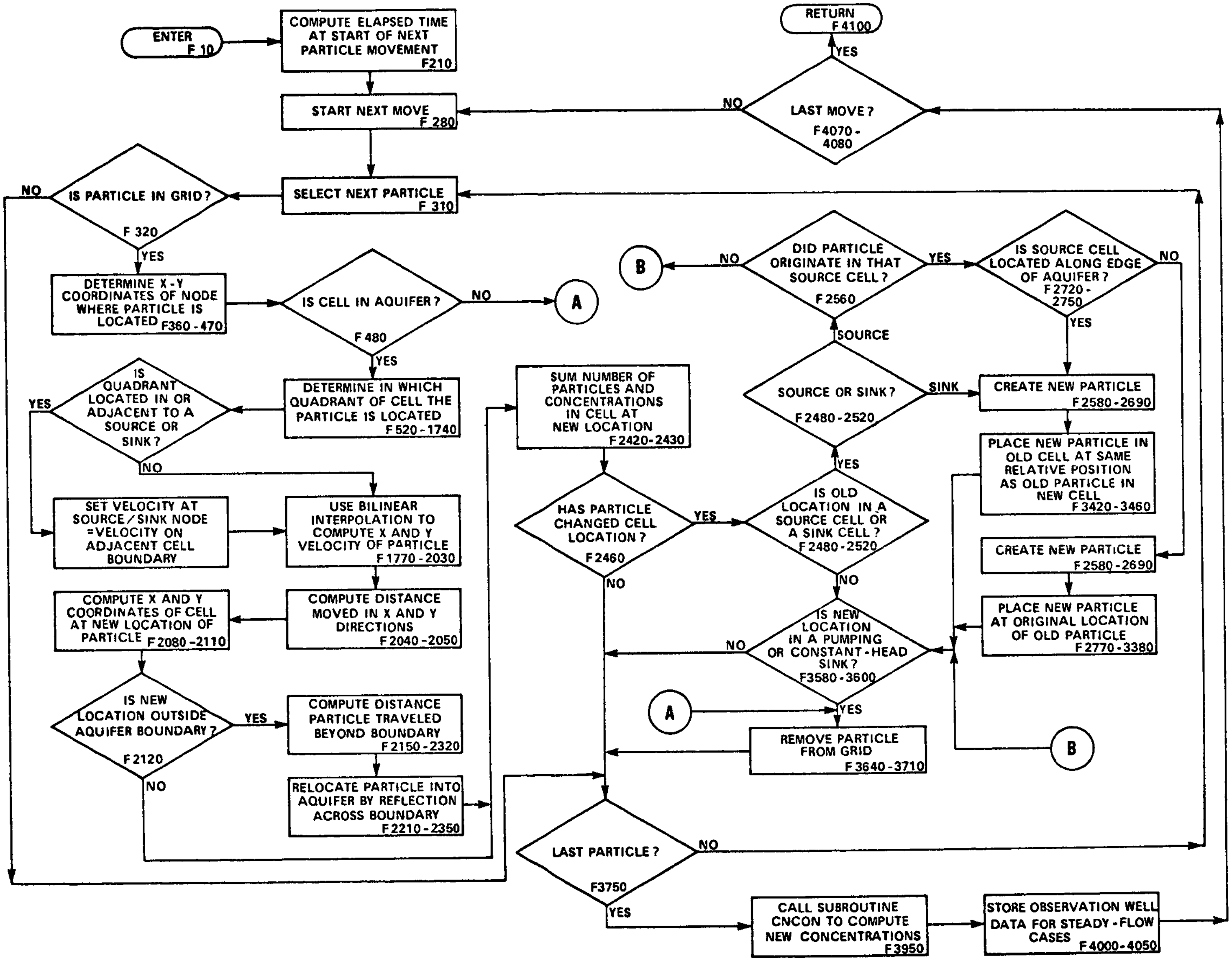


Figure 10.—Generalized flow chart of subroutine MOVE. Numbers indicate line numbers where the operation is executed.

at each node. If VPRM exceeds 0.09, it is assumed that the node represents a constant-head boundary condition and is treated as a fluid source or sink accordingly. At a constant-head node the difference in head between the aquifer and the source bed is used to determine whether the node represents a fluid source or sink (for example, lines F2500–F2520).

Subroutine CNCON

This subroutine computes the change in concentration at each node and at each particle for the given time increment. Equation 39, which denotes the change in concentration resulting from sources, divergence of velocity, and changes in saturated thickness, is solved on lines G350–G610. On the G520 the value of the storage coefficient is checked to determine whether the aquifer is confined or unconfined. It assumes that if $S<0.005$, then the aquifer is confined and $\partial b/\partial t=0$. If $S\geq 0.005$, the model assumes that $\partial b/\partial t = \partial h/\partial t$. If this criterion is not appropriate to a particular aquifer system, then line G520 should be modified accordingly. The change in concentration caused by hydrodynamic dispersion is computed on lines G640–G770 as indicated by equations 37 and 38.

The nodal changes in concentration caused by convective transport are computed on lines G850–G940. The number of cells that are void of particles at the new time level are also counted in this set of statements on lines G880–G910, and then compared with the critical number of void cells (NZCRIT) to determine if particles should be regenerated at initial positions before the next time level is started (lines G960–G1020).

The new (time level k) concentrations at nodes are computed on the basis of the previous concentration at time $k-1$ and the change during $k-1$ to k. The adjustment at nodes is accomplished on lines G1060–G1180, while the concentration of particles is adjusted on lines G1210–G1360.

A mass balance for the solute is next computed (lines G1400–G1730) at the end of each time increment. In computing the mass of solute withdrawn or leaking out of the aquifer at fluid sinks, the concentration at the sink node is assumed to equal the nodal concentration computed at time level $k-1$.

Subroutine OUTPT

This subroutine prints the results of the flow model calculations. When invoked, the subroutine prints (1) the new hydraulic head matrix (lines H190–H260), (2) a numeric map of head values (H300–H390), and (3) a drawdown map (H510–H710). This subroutine also computes a mass balance for the flow model and estimates its accuracy (H420–H820). A mass balance is performed both for cumulative volumes since the initial time and for flow rates during the present time step. The mass balance results are printed on lines H840–H930.

Subroutine CHMOT

This subroutine prints (1) maps of concentration (lines I250–I380), (2) change in concentration from initial conditions (I440–I580), and (3) the results of the cumulative mass balance for the solute (I670–I860). The accuracy of the chemical mass balance is estimated on lines I610–I660 using equations 62 and 64. The former is not computed if there was no change in the total mass of solute stored in the aquifer. The latter is not computed if the initial concentrations were zero everywhere. Lines I890–I1140 serve to print the head and concentration data recorded at observation wells. These data are recorded after each time step for a transient flow problem and after each particle movement for a steady-state flow problem. The data are printed after every 50 time increments and at the end of the simulation period.

Evaluation of Model

Comparison with analytical solutions

The accuracy of the numerical solution to the solute-transport equation can be evaluated in part by analyzing relatively simple problems for which analytical solutions are available and then comparing the numerical calculations with the analytical solution. Figure 11 presents such a comparison for a problem of one-dimensional steady-state flow through a homogeneous isotropic porous medium. The analytical solution is obtained with the following equation presented by Bear (1972, p. 627):

$$\frac{C(x,t)-C_0}{C_1-C_0}=\frac{1}{2}\text{erfc}\left\{-\frac{x-qt/\epsilon}{\sqrt{4D_Lt}}\right\} \quad (68)$$

where

erfc is the complimentary error function, and

$q=\epsilon V$ is the specific discharge, LT^{-1}.

Bear (1972, p. 627) shows that equation 68 is subject to the following initial conditions:

$$t\leq 0,\quad -\infty<x<0,\quad C=C_0$$
$$0\leq x<+\infty,\quad C=C_1$$

and to the following boundary conditions:

$$t>0,\quad x=\pm\infty,\quad \partial C/\partial x=0$$
$$x=+\infty,\quad C=C_1$$
$$x=-\infty,\quad C=C_0.$$

The general computer program presented in this report was modified in three simple ways for application to a problem equivalent to the one for which the analytical solution was derived. First, the program's arrays were redimensioned to 3 by 50 rather than 20 by 20. The aquifer (or column of porous medium) was thus represented by a 1-by-48 array of nodes. A grid spacing of 10 ft (3.05 m) was used. Second, the flow velocity was specified as a constant value, rather than being computed implicitly on the basis of hydraulic gradients and hydraulic conductivity. Third, the first (upstream) node of the aquifer was specified as a constant-concentration boundary, so that the concentration at node (2,2) was always equal to C_0 of

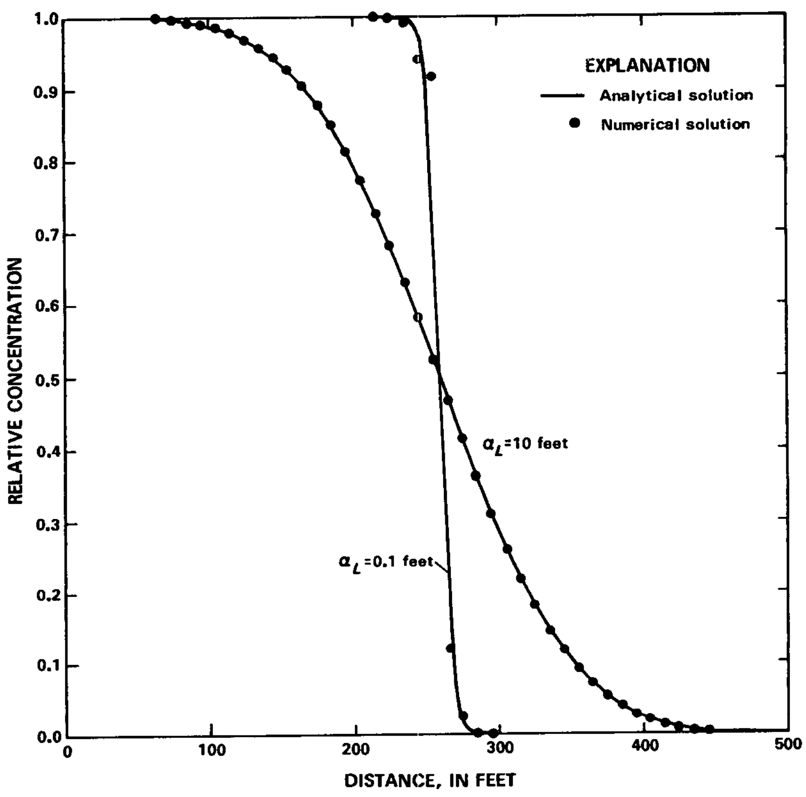


Figure 11.—Comparison between analytical and numerical solutions for dispersion in one-dimensional, steady-state flow.

equation 68. In the analysis of one-dimensional test problems, it was assumed that porosity equals 0.35, velocity equals 3.0×10^{-4} ft/s (9.1×10^{-5} m/s), and time equals 10.0 days.

As shown in figure 11, comparisons between the analytical and numerical solutions were made for two different values of dispersivity. For the higher dispersion there was essentially an exact agreement between the two curves. In the case of low dispersion, there is a very small difference at some nodes between the concentrations computed analytically and those computed numerically. This difference is caused primarily by the error in computing the concentration at a node as the arithmetic average of the concentrations of all particles located in that cell. This is not considered to be a serious problem since this error is not cumulative. Also note in the case of low dispersion that the grid spacing (10 ft or 3.05 m) was coarse relative to the width of the breakthrough curve between concentrations of 0.05 and 0.95. Nevertheless, the numerical model still accurately computed the shape and position of the front.

In computing the numerical solutions shown in figure 11 the program was executed using nine particles per cell and with CELDIS=0.50 (γ in equations 54–55). The 10-day simulation required 52 time increments and used about 40 seconds of cpu on a Honeywell 60/68 computer.

An analytical solution is also available for the problem of plane radial flow in which a well continuously injects a tracer at constant rate q_w and constant concentration C_0. Bear (1972, p. 638) indicates that the following equation is appropriate for this problem (although there are some limitations discussed by Bear):

$$\frac{C}{C_0}=\frac{1}{2}\text{erfc}\left\{\frac{r^2/2-Gt}{\sqrt{4/3\alpha_1\bar{r}^3}}\right\} \tag{69}$$

where

G $=\dfrac{q_w}{2\pi\epsilon b}=Vr;$

r is the radial distance from the center of the well, L; and

$\bar{r}=(2Gt)^{1/2}$ is the average radius of the body of injected water, L.

Again, the general computer program had to be somewhat modified to permit a suitable comparison to be made between the analytical solution and the numerical model. One change involved the direct calculation of velocity at any point based on its distance from the well using the following equation:

$$V=\frac{q_w}{2\pi r\epsilon b}. \tag{70}$$

The other significant change was made in subroutine GENPT to allow the initial placement of 16 particles per cell, rather than the present maximum of 9. In the analysis of test problems for radial flow, it was assumed that porosity equals 0.35, the injection rate (q_w) equals 1.0 ft^3/s (0.028 m^3/s), saturated thickness equals 10.0 ft (3.05 m), and longitudinal dispersivity equals 10.0 ft (3.05 m).

The application of the method of characteristics, which was written for two-dimensional Cartesian coordinates, to a problem involving radially symmetric divergent flow represents a severe test of the model. Nevertheless, it can be seen in figure 12 that there is good agreement between the analytical and numerical solutions after both relatively short and long times. However, the presence of some numerical dispersion is evident, particularly for the longer time. The numerical dispersion is introduced in part during the regeneration of particles after the number of cells void of particles has exceeded the critical number. The geometry of initial particle placement minimized this problem in cells that lay in the same row or column of the grid as the injection well. The circles in figure 12, which indicate concentration values computed at these nodes, agree closely with the analytical solution. The greatest errors occur at nodes on radii from the injection well that are neither parallel to nor 45° from the main axes of the grid. These results indicate that this Cartesian coordinate model is not best suited for application to purely radial flow problems. However, if radially divergent flow is limited to areas of several

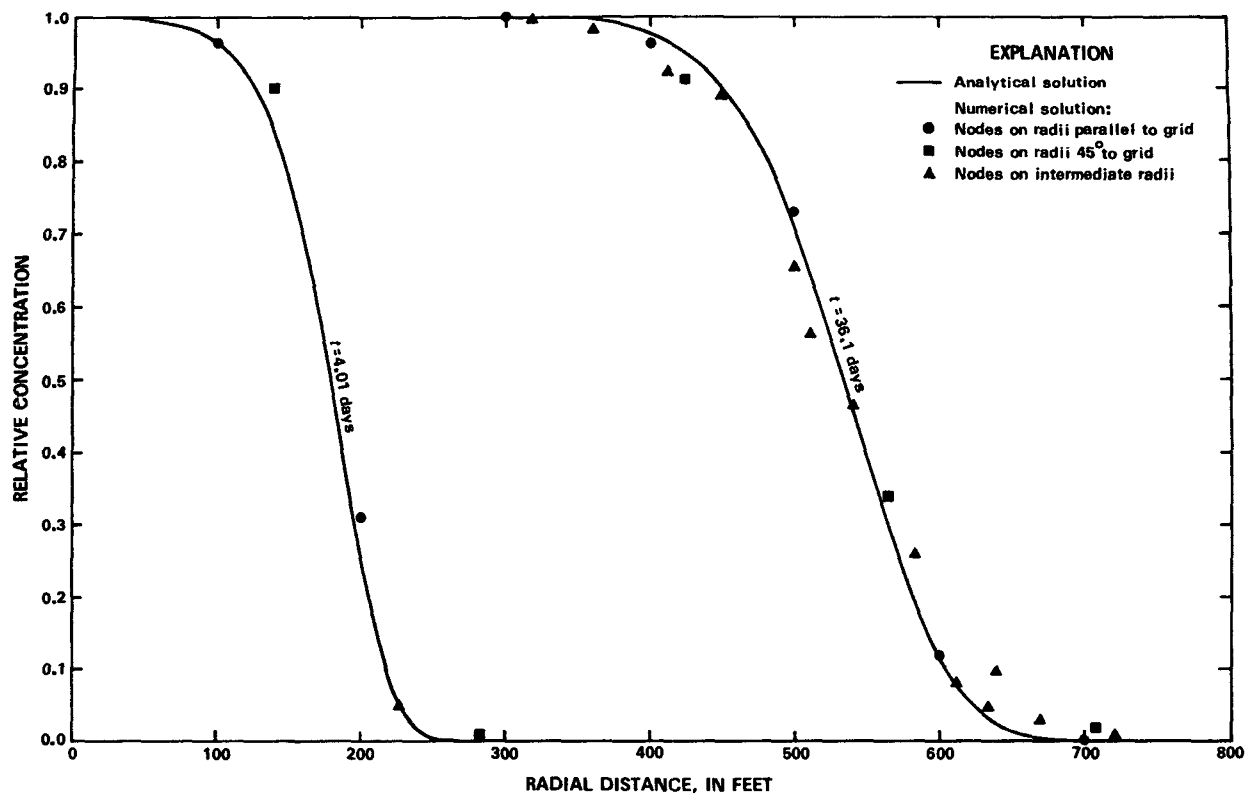


Figure 12.—Comparison between analytical and numerical solutions for dispersion in plane radial steady-state flow.

rows and columns within a more uniform regional flow field, the model will accurately compute concentration distributions. To apply the method of characteristics to a problem of plane radial flow, it would be best to rewrite the program in a system of radial coordinates, which should improve the accuracy for those problems to the same order shown in figure 11 for the analysis of one-dimensional flow.

Mass balance tests

The accuracy and precision of the numerical solution can also be partly evaluated by computing the magnitude of the error in the mass balance. The mass balance error will depend on the nature of the problem and will vary from one time step to the next. During the development of the program, the model was applied to a variety of hypothetical solute-transport problems to assure its flexibility, transferability, and accuracy under a wide range of conditions. To illustrate the range in mass balance errors that might be expected and some of the factors that affect it, several of these problems are presented here.

Test problem 1—spreading of a tracer slug

The first test described here was designed to evaluate the accuracy of simulating the processes of convective transport and dispersion independent of the effects of chemical sources. Thus, a slug of tracer was initially placed in four cells of a grid whose boundary conditions generated a steady-state flow field that was moderately divergent in some places and moderately convergent in other places, as illustrated in figure 13. The aquifer was assumed to be homogeneous and isotropic. Because flow was assumed to be in steady state, the storage coefficient was set equal to 0.0. The parameters used to define problem

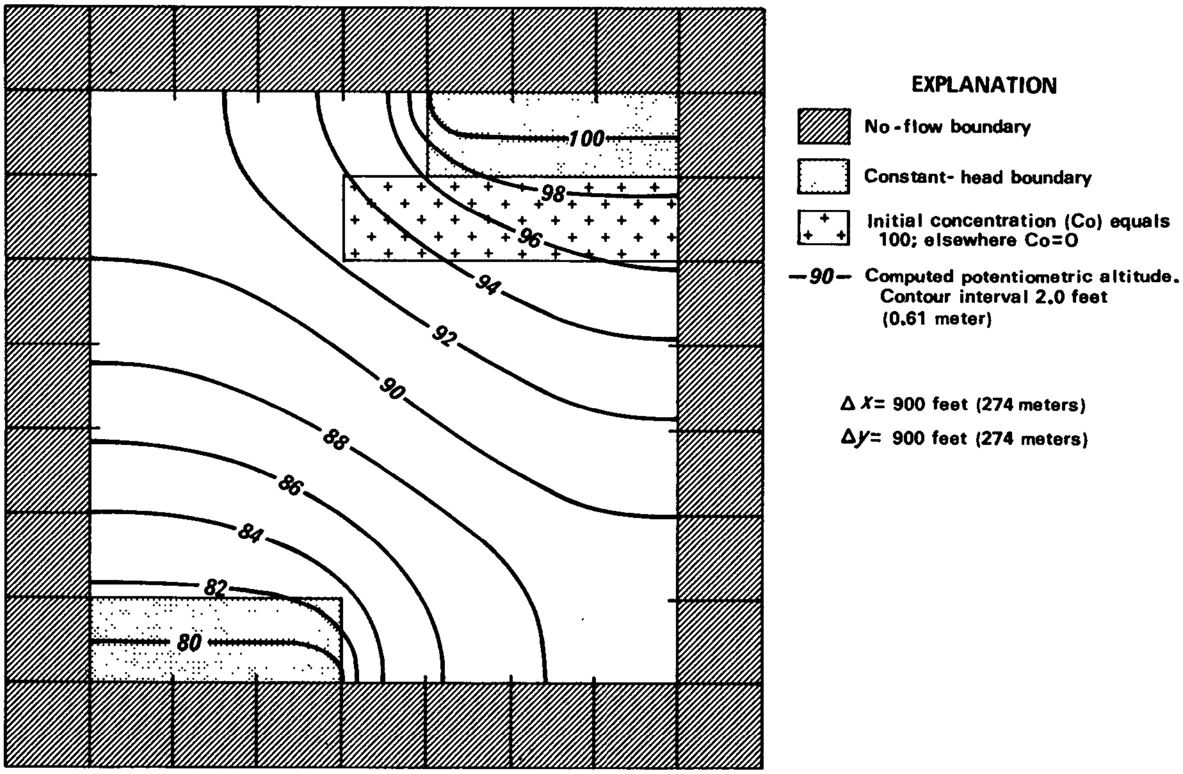


Figure 13.—Grid, boundary conditions, and flow field for test problem 1.

1 are listed in table 2. The slug of known mass was then allowed to spread downgradient for a period of 2.0 years.

Table 2.—Model parameters for test problem 1

Aquifer properties	Numerical parameters
K=0.005 ft/s (1.5×10^{-3} m/s)	Δx=900 ft (274 m)
b=20.0 ft (6.1 m)	Δy=900 ft (274 m)
S=0.0	CELDIS=0.49
ε=0.30	NPTPND=9
α_T/α_L=0.30	

The model first computed a steady-state head distribution, shown in figure 13, and velocity field. The model required 12 time increments (or particle movements) to simulate a 2.0-year period. The model was run to simulate conditions of no dispersion (α_L=0.0 ft) as well as moderate dispersion (α_L=100 ft or 30.5 m). The mass balance error computed using equation 64 is shown in figure 14 for both conditions. In these tests the error averages 1.9 percent and is always within a range of ±8 percent. Much of the error is related to the calculation of nodal concentrations based on the arithmetic mean of particle concentrations in each cell. When a particle moves across a cell boundary, its area of influence shifts entirely from the first node to the second. Thus, depending on the local density of points and local concentration gradients, the use of an arithmetic mean to compute nodal concentrations may give too much weight to some particles and too little weight to others. The use of a weighted mean, in which the weighting factor is a function of the distance between a node and a particle, reduced the error to some degree. But the improvement in precision was small compared with the increase in computational requirements, so this algorithm was not included in the general program. Because the error caused by using an arithmetic mean is not cumulative, it is not considered a serious

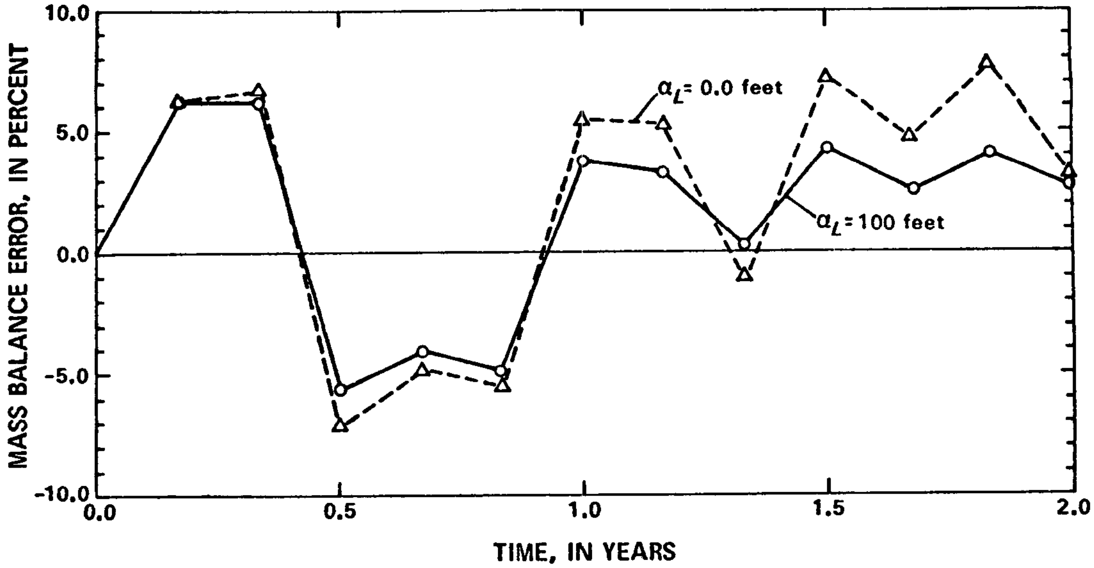


Figure 14.—Mass balance errors for test problem 1.

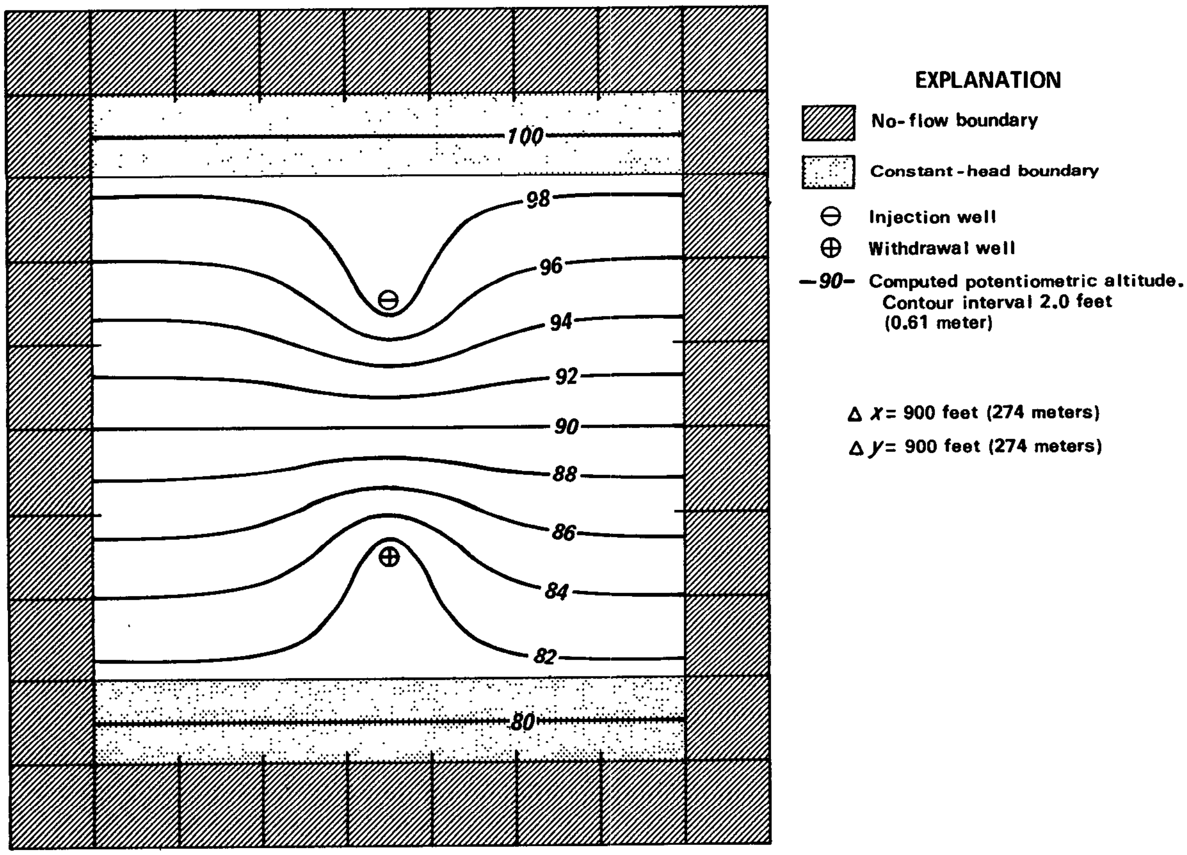


Figure 15.—Grid, boundary conditions, and flow field for test problem 2.

problem. Furthermore, figure 14 shows that the error decreases for a higher dispersivity because dispersion smooths out sharp fronts and minimizes strong concentration gradients.

Test problem 2—effects of wells

The second problem was designed to evaluate the application of the model to problems in which the flow field is strongly influenced by wells. The grid and boundary conditions used to define this problem are illustrated in figure 15. The problem consists of one injection well and one withdrawal well, whose effects are superimposed on a regional flow field controlled by two constant-head boundaries. The parameters for problem 2 are defined in table 3. The aquifer was also assumed to be homogeneous and isotropic. The model simulated a period of 2.4 years and assumed steady-state flow.

The model required 18 time increments (or particle movements) to simulate a 2.4-year period of solute transport. Problem 2 was also evaluated for conditions of no dispersion (α_L=0.0 ft) as well as moderate dispersion (α_L=100 ft or 30.5 m). The mass balance error was computed using equation 62 and is shown in figure 16 for both conditions. The average of the 36 values shown in figure 16 is −0.06 percent; the error always falls within the range of ±8 percent. It can be seen that in this case the errors are essentially coincident for almost 1 year, after which the error appears to be dependent on the magnitude of dispersion. However, the model output showed that when α_L=100 ft (30.5 m), the leading edge of the breakthrough curve (or chemical front) reaches the constant-head sink just prior to 1.0 year. When α_L=0.0 ft, the leading edge of the breakthrough curve still had not entered the constant-head sink after 2.4 years. Because the two curves in figure 16 are essentially coincident prior to 1.0 year, it thus appears that the divergence of the two curves is not caused directly by the difference in dispersivity. Rather, it is related to the difference in arrival times at the hydraulic sinks and is a direct effect of the manner in which con-

Table 3.—Model parameters for test problems 2 and 3

Aquifer properties and stresses	Numerical parameters
K=0.005 ft/s (1.5×10^{-3} m/s)	Δx=900 ft (274 m)
b=20.0 ft (6.1 m)	Δy=900 ft (274 m)
S=0.0	CELDIS=0.50
ε=0.30	NPTPND=9
α_T/α_L=0.30	
C'=100.0	
C_0=0.0	
q_w=1.0 ft^3/s (0.028 m^3/s)	

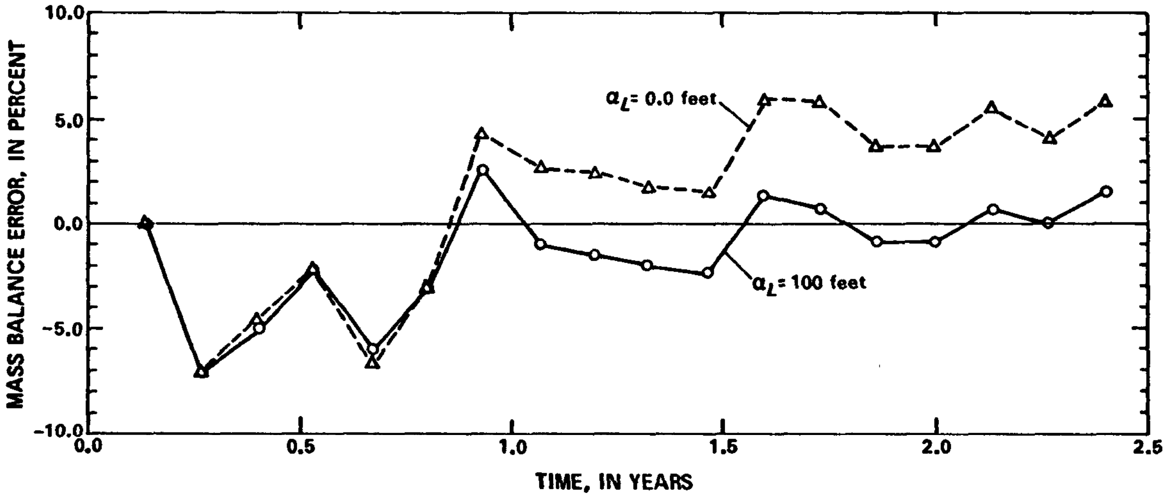


Figure 16.—Mass balance errors for test problem 2.

centrations are computed at sink nodes and (or) the method of estimating the mass of solute removed from the aquifer at sink nodes during each time increment.

Test problem 3—effects of user options

In addition to the input options that control the form or frequency of the output, there are two execution parameters that must be specified by the user and influence the accuracy, precision, and efficiency (or computational cost) of the solution to a particular problem. These execution parameters are the initial number of particles per node (NPTPND) and the maximum fraction of the grid dimensions that particles are allowed to move (γ in equations 54–55 or CELDIS in the program). The third test problem was designed to allow an evaluation of both of these parameters. As illustrated in figure 17, this problem consists of one withdrawal well located in a regional flow field that is controlled by two constant-head boundaries. The contamination sources are three central nodes along the upgradient constant-head boundary. The model parameters for test problem 3 are the same as for test problem 2, as listed in table 3. However, for test problem 3 solutions were obtained using a range in values for CELDIS and NPTPND.

The solution to this problem was found to be sensitive to the density of tracer particles used in the simulation. Figure 18 shows how the error in the mass balance varied with time for cases of NPTPND equal to 4, 5, 8, and 9. Table 4 lists the execution time and the mean and standard deviation of the mass balance error for each case. These data clearly indicate that the accuracy and precision

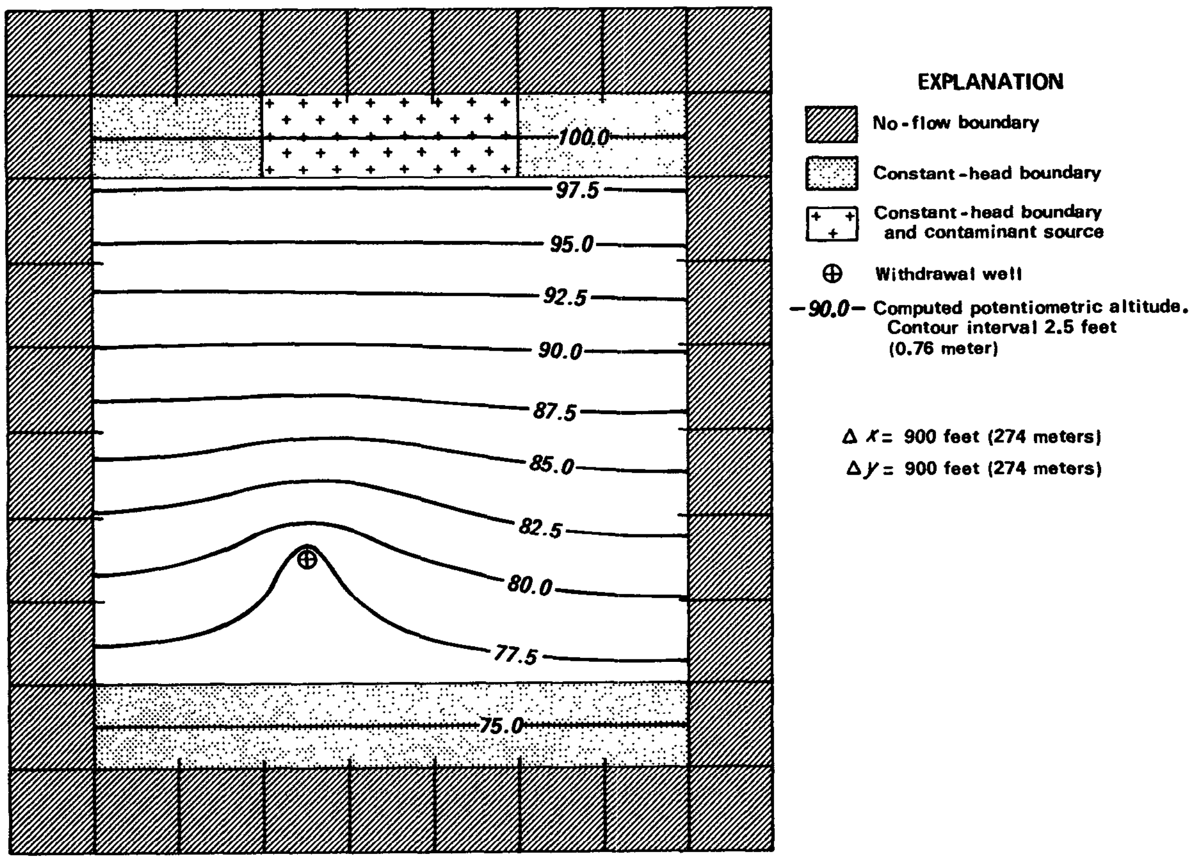


Figure 17.—Grid, boundary conditions, and flow field for test problem 3.

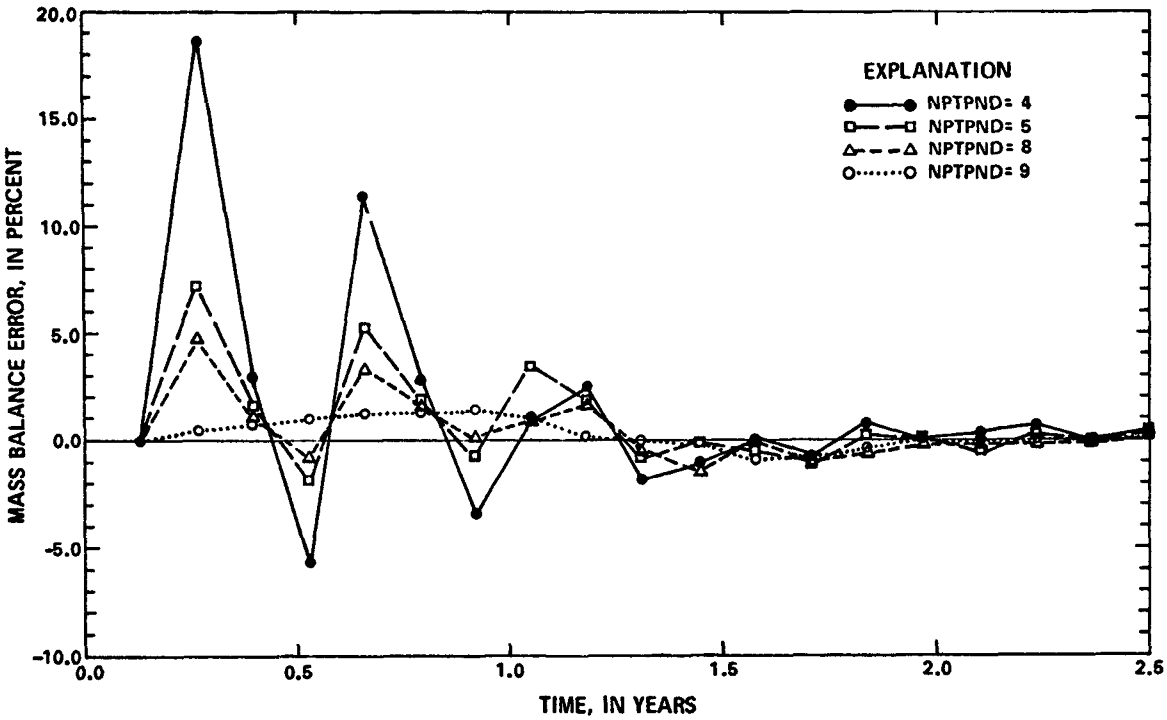


Figure 18.—Effect of NPTPND on mass balance error for test problem 3; CELDIS=0.50 in all cases.

Table 4.—Effect of NPTPND on accuracy, precision, and efficiency of solution to test problem 3

NPTPND	cpu-seconds [1]	Mass balance error (percent) Mean	Standard deviation
4	12.8	1.49	5.33
5	14.0	.90	2.29
8	17.9	.48	1.53
9	19.2	.26	.69

[1] The program was executed on a Honeywell 60/68 computer; CELDIS=0.50.

of the solution are directly proportional to particle density, while the efficiency of the solution is inversely related to NPTPND. In other words, a better solution will cost more. It is important to note that the oscillations or scatter shown in figure 18 decrease with time and that there is essentially no difference among the solutions and among the mass balance errors for times greater than about 1.5 years.

Next the effect of CELDIS (or γ) was evaluated for test problem 3 by setting NPTPND=9 and running the model with several possible values of CELDIS. Figure 19 shows how the error in the mass balance varied with time for cases of CELDIS equal to 0.25, 0.50, 0.75, and 1.00. Table 5 lists the execution time and the mean and standard deviation of the mass balance error for each case. These data indicate that the relationship between CELDIS and the mass balance error is not as simple and straightforward as for NPTPND. It is apparent that the results for 0.50, 0.75, and 1.00 are similar, and of these, the results for CELDIS=0.50 ap-

Table 5.—Effect of CELDIS on accuracy, precision, and efficiency of solution to test problem 3

CELDIS	cpu-seconds [1]	Mass balance error (percent) Mean	Standard deviation
0.25	34.6	1.50	2.99
.50	19.2	.26	.69
.75	14.4	.56	.69
1.00	12.1	.25	1.48

[1] The program was executed on a Honeywell 60/68 computer; NPTPND=9.

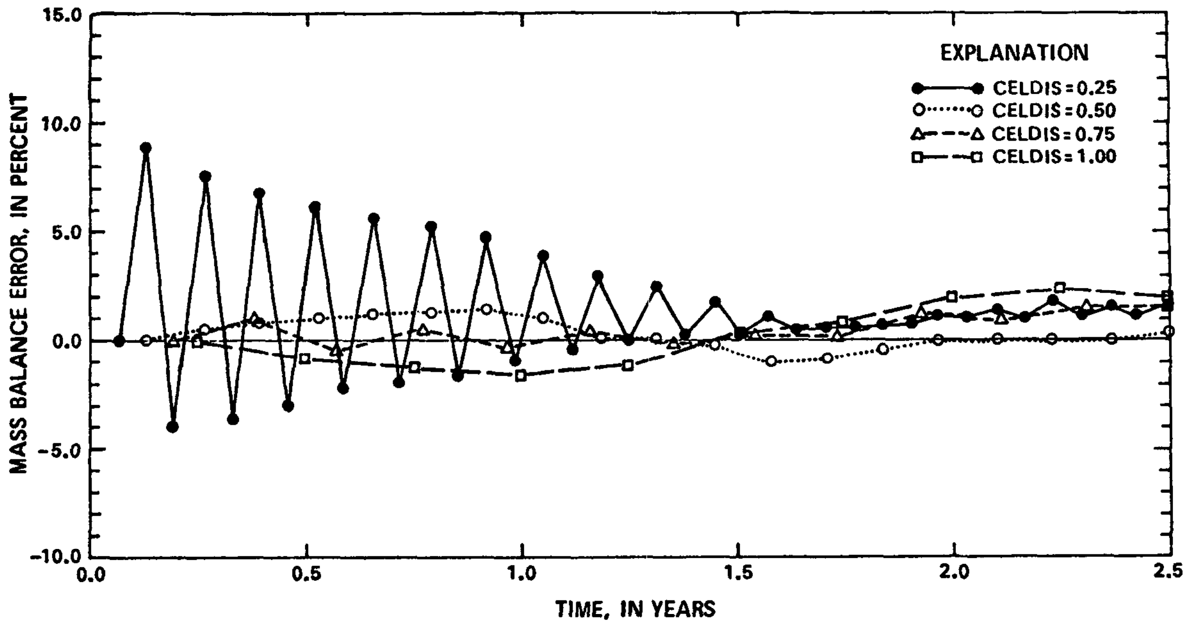


Figure 19.—Effect of CELDIS on mass balance error for test problem 3; NPTPND=9 in all cases.

pear to be the best. However, when CELDIS was reduced to 0.25, the error oscillated strongly for about 1.5 years before apparently converging to a small error within the range of the other curves. This oscillation occurred because the maximum distance a particle could move (25 percent of the grid dimensions) was less than the spacing between particles (33 percent of the grid dimensions for NPTPND=9). Thus, convective transport across the boundaries of cells could not be adequately represented for any single time step in those parts of the grid where the concentration was changing significantly with time. But over two successive time increments the error would average out to a minimum. As the contaminated area increases in size over time, the error in computed concentrations at cells near the front (that is, in areas of steep concentration gradient) becomes an increasingly smaller percentage of the total mass of solute present in the aquifer. Hence, the mass balance error generally tends to approach a minimal range with time for these types of problems.

The effects of NPTPND and CELDIS on the mass balance error are problem dependent. In problems for which CELDIS is not the limiting stability criterion, varying CELDIS will have no effect on the solution. Because of the possible tradeoff between accuracy and efficiency, it is recommended in general that the model user specify NPTPND as 4 or 5 and CELDIS as 0.75 to 1.0 for runs made during the early stages of model calibration when frequent runs are made and maximum efficiency is desired. For final runs when maximum accuracy is desired, set NPTPND equal to 9 and CELDIS equal to 0.50.

Possible program modifications

The program presented here represents a basic and general solute-transport model. Some program modifications may be desirable or even necessary to allow the model to be applied efficiently to a particular field problem. Some changes might require only minor adjustments, while others might involve major rewriting of the program. The purpose of this section is to discuss some of the modifications that might commonly be considered, and that might be incorporated into the present basic model, rather than using an entirely different solution technique.

Coordinate system and boundary conditions

After the finite-difference grid is designed, the first program modification that should be made is to modify the array dimensions for the specific grid used. This will permit the most efficient use of computer storage. The array sizes should be set equal to NX, NY, and NPMAX, which are specified on Input Card 2. The maximum number of particles, NPMAX, may be computed from the following equation:

$$NPMAX \cong (NX-2)(NY-2)(NPTPND) + (N_s)(NPTPND) + 250 \quad (71)$$

where

N_s is the number of nodes that represent fluid sources, either at wells or at constant-head cells.

The values of NX and NY should be substituted for the 20-by-20 arrays contained in COMMON statements PRMK, HEDA, HEDB, CHMA, CHMC, and DIFUS, and in DIMENSION statements on lines C170, G200, H140, and I160. The value of NPMAX should replace 3200 in the PART array in all the CHMA COMMON statements.

Although this program is designed for application to two-dimensional areal flow problems, it can be applied directly to two-dimensional cross sections. In this case the z-coordinate would replace the y-coordinate. Then the user would have to assume and specify unit width (THCK array) for Δy and substitute hydraulic conductivity for transmissivity in data set 3 of attachment III. If the problem involves transient flow, then specific storage (S_s) should be substituted for the storage coefficient. Also, if recharge or discharge is to be specified through the RECH array (data set 5), values should be divided by the thickness of the layer (Δz) to reduce the dimensionality of the stress rate to (T^{-1}) rather than (LT^{-1}) as indicated in the documentation. In applying the cross-sectional model to a field problem it is important that conditions meet the inherent assumption that there exist no significant components of flow into or out of the plane of the section. Because this assumption would probably be impossible to meet in the vicinity of a pumping well, the use of the REC array (data set 2) should usually be limited to representing special or known-flux boundary conditions.

The program can also be applied directly and simply to one-dimensional problems. In this case one of the dimensions (NX or NY) should be reduced to a value of 3, of which the outer two are used to represent the no-flow boundaries around the one-dimensional row or column.

The most complex type of change would involve rewriting the program for application to other than a two-dimensional rectangular grid. One possibility includes problems of flow to or from wells in which radial symmetry can be assumed. This would allow variables to be expressed in terms of r-z coordinates. Another possibility is to simulate three-dimensional flow in x-y-z coordinates. A three-dimensional finite-difference flow model is available (Trescott, 1975) and would be compatible with the method-of-characteristics solution to the solute-transport equation.

It is sometimes convenient to separately associate certain parts of the grid or certain boundary conditions with corresponding field conditions or hydrologic units. The analysis of flow patterns and water-quality changes may then be aided by performing separate mass balances (or budgets) for each characteristic type of node. The nodal types or zones can be conveniently identified through the NODEID array. Then the mass balance routines in subroutines CNCON and (or) OUTPT would have to be modified to tally fluxes separately for each NODEID; for an example, see Konikow (1977). Similarly, if a coupled stream-aquifer system is being considered, a separate subroutine may be added to route streamflow downstream and progressively account for ground-water gains and losses and for tributary inflow or diversions. An example of such a modification is discussed by Konikow and Bredehoeft (1974).

For certain types of problems it may be desirable to be able to specify a constant-concentration boundary condition. The program could be modified to allow this by using a predetermined value or range in values of NODEID to identify this type of boundary. Then a statement could be added between lines G1090 and G1100 to reset the concentration at the node equal to the constant concentration where this condition is specified. The value of the constant concentration can be stored in the CNRECH array. Note that the mass balance calculation as presently written will not account for the mass of solute added or removed at a constant-concentration boundary.

Basic equations

The basic equations that are solved by this model were derived under a number of limiting assumptions. Some of these assumptions can be overcome through modifications of the basic equations and corresponding changes in the program.

The program assumes that molecular diffusion is negligible. But if it is necessary to consider the process of molecular diffusion in a particular problem, the coefficient of hydrodynamic dispersion (D_{ij}) can be redefined as the sum of the coefficient of mechanical dispersion, which is defined by the right side of equation 5, and a coefficient of molecular diffusion. The consequent program modification would have to be made only in subroutine VELO (lines E1280–E1680).

The solute-transport equation can also be modified to include the effects of first-order chemical reactions, as was done by Robertson (1974). The reaction term could be included in the right side of equation 39. The corresponding program modification would be required in subroutine CNCON.

In certain problems the range in concentrations may be so great that the dependence of fluid properties, such as density and viscosity, on the concentration may have to be considered because of the dependence of fluid flow on variations in fluid properties. In this case the flow equation (eq 1) would have to be rewritten in terms of fluid pressure, rather than hydraulic head, such as equation 15 of Bredehoeft and Pinder (1973, p. 197). Then the program can be modified to iterate between the solutions to the flow and solute-transport equations if the change in fluid properties at any node exceeds some criterion during one time increment.

The flow equation can also be modified for application to unconfined aquifers in which the saturated thickness is a direct function of water-table elevation. This would require the inclusion of steps in subroutine ITERAT to correct the transmissivity for changes in saturated thickness. Such a feature is included in the two-dimensional flow model documented by Trescott, Pinder, and Larson (1976).

Input and output

The input and output formats have been designed for flexibility of use and general compatibility with the analysis of a variety of types of flow problems. If any of the formats are not suitable for use with a particular problem, they should be modified accordingly. All input formats are described in attachment III and contained in subroutine PARLOD in the program.

It has been assumed that several aquifer parameters are constant and uniform in space, such as storage coefficient, effective porosity, and dispersivity. If any of these are known to vary in space, they should be redefined as two-dimensional arrays. Then statements to allow these arrays to be read into the program should be added to subroutine PARLOD. Similarly, values of leakance and source concentrations (CNRECH) are only read in data set 7, where values can be associated only with a limited number of unique node identification codes. If the variations of these parameters are known on a more detailed scale, then they too can be read as additional data sets by adding appropriate statements to subroutine PARLOD. For example, a typical sequence of statements for reading one data set is represented by lines B2650–B2750, where the initial water-table elevations (data set 8) are read. This sequence of statements can then be replicated for reading in a different data set and inserted into subroutine PARLOD.

A labeled listing of the input data deck for test problem 3 is provided in attachment IV. This example illustrates the use of the data input formats specified in attachment III and shows that only a few data cards are required by the model to simulate a relatively simple problem. This example will also allow the user to verify that his program deck and computer yield essentially the same results as obtained by the documented program. Thus, selected parts of the output for test problem 3 are included in attachment V. Not all of the printed output from test problem 3 has been duplicated in attachment III. Instead, it contains only a sufficient selection to illustrate the type and form of output provided by the model, as well as to allow the user to compare his calculated values of critical parameters, such as head, velocity, and concentration, with the values computed by the documented model.

Conclusions

The model presented in this report can simulate the two-dimensional transport and dispersion of a nonreactive solute in either steady-state or transient ground-water flow. The program is general and flexible in that it can be readily and directly applied to a wide range of types of problems, as defined by aquifer properties, boundary conditions, and stresses. However, some program modifications may be required for application to specialized problems or conditions not included in the general model.

The accuracy of the numerical results can be evaluated by comparison with analytical solutions only for relatively simple and idealized problems; in these cases there was good agreement between the numerical and analytical results. Mass balance tests also help to evaluate the accuracy and precision of the model results. The error in the mass balance is generally less than 10 percent. The range in mass balance errors is commonly the greatest during the first few time increments, but tends to decrease and stabilize with time. For some problems the accuracy and precision of the numerical results may be sensitive to the initial number of particles placed in each cell and to the size of the time increments, as determined by the stability criteria for the solute-transport equation. The results of several numerical experiments suggest that the accuracy and precision of the results are essentially independent of the magnitude of the dispersion coefficient, and comparable accuracies are attained for high, low, or zero dispersivities.

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Robertson, J. B., 1974, Digital modeling of radioactive and chemical waste transport in the Snake River Plain aquifer at the National Reactor Testing Station, Idaho: U.S. Geol. Survey Open-File Rept. IDO-22054, 41 p.

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Scheidegger, A. E., 1961, General theory of dispersion in porous media: Jour. Geophys. Research, v. 66, no. 10, p. 3273-3278.

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COMPUTER PROGRAM AND RELATED DATA

Attachment I

FORTRAN IV Program Listing

```
C     *****************************************************************
C     *                                                               *
C     *      SOLUTE TRANSPORT AND DISPERSION IN A POROUS MEDIUM       *
C     *       NUMERICAL SOLUTION --- METHOD OF CHARACTERISTICS        *
C     *       PROGRAMMED BY J. D. BREDEHOEFT AND L. F. KONIKOW        *
C     *                                                               *
C     *****************************************************************
      DOUBLE PRECISION DMIN1,DEXP,DLOG,DABS
      REAL *8TMRX,VPRM,HI,HR,HC,HK,WT,REC,RECH,TIM,AOPT,TITLE
      REAL *8XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      REAL *8TINT,ALPHA1,ANITP
      COMMON /PRMI/ NTIM,NPMP,NPNT,NITP,N,NX,NY,NP,NREC,INT,NNX,NNY,NUMO
     1BS,NMOV,IMOV,NPMAX,ITMAX,NZCRIT,IPRNT,NPTPND,NPNTMV,NPNTVL,NPNTD,N
     2PNCHV,NPDELC
      COMMON /PRMK/ NODEID(20,20),NPCELL(20,20),LIMBO(500),IXOBS(5),IYOB
     1S(5)
      COMMON /HEDA/ THCK(20,20),PERM(20,20),TMWL(5,50),TMOBS(50),ANFCTR
      COMMON /HEDB/ TMRX(20,20,2),VPRM(20,20),HI(20,20),HR(20,20),HC(20,
     120),HK(20,20),WT(20,20),REC(20,20),RECH(20,20),TIM(100),AOPT(20),T
     2ITLE(10),XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /CHMA/ PART(3,3200),CONC(20,20),TMCN(5,50),VX(20,20),VY(20,
     120),CONINT(20,20),CNRECH(20,20),POROS,SUMTCH,BETA,TIMV,STORM,STORM
     2I,CMSIN,CMSOUT,FLMIN,FLMOT,SUMIO,CELDIS,DLTRAT,CSTORM
C     ****************************************************************
C       ---LOAD DATA---
      INT=0
      CALL PARLOD
      CALL GENPT
C     ****************************************************************
C     ---START COMPUTATIONS---
C        ---COMPUTE ONE PUMPING PERIOD---
      DO 150 INT=1,NPMP
      IF (INT.GT.1) CALL PARLOD
C        ---COMPUTE ONE TIME STEP---
      DO 130 N=1,NTIM
      IPRNT=0
C        ---LOAD NEW DELTA T---
      TINT=SUMT-PYR*(INT-1)
      TDEL=DMIN1(TIM(N),PYR-TINT)
      SUMT=SUMT+TDEL
      TIM(N)=TDEL
      REMN=MOD(N,NPNT)
C     ****************************************************************
      CALL ITERAT
      IF (REMN.EQ.0.0.OR.N.EQ.NTIM) CALL OUTPT
      CALL VELO
      CALL MOVE
C     ****************************************************************
C     ---STORE OBS. WELL DATA FOR TRANSIENT FLOW PROBLEMS---
      IF (S.EQ.0.0) GO TO 120
      IF (NUMOBS.LE.0) GO TO 120
      J=MOD(N,50)
      IF (J.EQ.0) J=50
      TMOBS(J)=SUMT
      DO 110 I=1,NUMOBS
      TMWL(I,J)=HK(IXOBS(I),IYOBS(I))
      TMCN(I,J)=CONC(IXOBS(I),IYOBS(I))
  110 CONTINUE
```

FORTRAN IV program listing—Continued

```
C     ******************************************************************
C     ---OUTPUT ROUTINES---
  120 IF (REMN.EQ.0.0.OR.N.EQ.NTIM.OR.MOD(N,50).EQ.0) CALL CHMOT
      IF (SUMT.GE.(PYR*INT)) GO TO 140
  130 CONTINUE
C     ******************************************************************
C     ---SUMMARY OUTPUT---
  140 CONTINUE
      IPRNT=1
      CALL CHMOT
  150 CONTINUE
C     ******************************************************************
      STOP
C     ******************************************************************
      END
      SUBROUTINE PARLOD
      DOUBLE PRECISION DMIN1,DEXP,DLOG,DABS
      REAL *8TMRX,VPRM,HI,HR,HC,HK,WT,REC,RECH,TIM,AOPT,TITLE
      REAL *8XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      REAL *8FCTR,TIMX,TINIT,PIES,YNS,XNS,RAT,HMX,HMY
      REAL *8TINT,ALPHA1,ANITP
      COMMON /PRMI/ NTIM,NPMP,NPNT,NITP,N,NX,NY,NP,NREC,INT,NNX,NNY,NUMO
     1BS,NMOV,IMOV,NPMAX,ITMAX,NZCRIT,IPRNT,NPTPND,NPNTMV,NPNTVL,NPNTD,N
     2PNCHV,NPDELC
      COMMON /PRMK/ NODEID(20,20),NPCELL(20,20),LIMBO(500),IXOBS(5),IYOB
     1S(5)
      COMMON /HEDA/ THCK(20,20),PERM(20,20),TMWL(5,50),TMOBS(50),ANFCTR
      COMMON /HEDB/ TMRX(20,20,2),VPRM(20,20),HI(20,20),HR(20,20),HC(20,
     120),HK(20,20),WT(20,20),REC(20,20),RECH(20,20),TIM(100),AOPT(20),T
     2ITLE(10),XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /CHMA/ PART(3,3200),CONC(20,20),TMCN(5,50),VX(20,20),VY(20,
     120),CONINT(20,20),CNRECH(20,20),POROS,SUMTCH,BETA,TIMV,STORM,STORM
     2I,CMSIN,CMSOUT,FLMIN,FLMOT,SUMIO,CELDIS,DLTRAT,CSTORM
      COMMON /BALM/ TOTLQ
      COMMON /XINV/ DXINV,DYINV,ARINV,PORINV
      COMMON /CHMC/ SUMC(20,20),VXBDY(20,20),VYBDY(20,20)
C     ******************************************************************
      IF (INT.GT.1) GO TO 10
      WRITE (6,750)
      READ (5,720) TITLE
      WRITE (6,730) TITLE
C     ******************************************************************
C     ---INITIALIZE TEST AND CONTROL VARIABLES---
      STORMI=0.0
      TEST=0.0
      TOTLQ=0.0
      SUMT=0.0
      SUMTCH=0.0
      INT=0
      IPRNT=0
      NCA=0
      N=0
      IMOV=0
      NMOV=0
C     ******************************************************************
C     ---LOAD CONTROL PARAMETERS---
      READ (5,740) NTIM,NPMP,NX,NY,NPMAX,NPNT,NITP,NUMOBS,ITMAX,NREC,NPT
     1PND,NCODES,NPNTMV,NPNTVL,NPNTD,NPDELC,NPNCHV
      READ (5,800) PINT,TOL,POROS,BETA,S,TIMX,TINIT,XDEL,YDEL,DLTRAT,CEL
     1DIS,ANFCTR
      PYR=PINT*86400.0*365.25
      NNX=NX-1
```

FORTRAN IV program listing—Continued

```
      NNY=NY-1
      NP=NPMAX
      DXINV=1.0/XDEL
      DYINV=1.0/YDEL
      ARINV=DXINV*DYINV
      PORINV=1.0/POROS
C     ---PRINT CONTROL PARAMETERS---
      WRITE (6,760)
      WRITE (6,770) NX,NY,XDEL,YDEL
      WRITE (6,780) NTIM,NPMP,PINT,TIMX,TINIT
      WRITE (6,790) S,POROS,BETA,DLTRAT,ANFCTR
      WRITE (6,870) NITP,TOL,ITMAX,CELDIS,NPMAX,NPTPND
      IF (NPTPND.LT.4.OR.NPTPND.GT.9.OR.NPTPND.EQ.6.OR.NPTPND.EQ.7) WRIT
     1E (6,880)
      WRITE (6,890) NPNT,NPNTMV,NPNTVL,NPNTD,NUMOBS,NREC,NCODES,NPNCHV,N
     1PDELC
      IF (NPNTMV.EQ.0) NPNTMV=999
      GO TO 20
C     ******************************************************************
C     ---READ DATA TO REVISE TIME STEPS AND STRESSES FOR SUBSEQUENT
C        PUMPING PERIODS---
   10 READ (5,1060) ICHK
      IF (ICHK.LE.0) RETURN
      READ (5,1070) NTIM,NPNT,NITP,ITMAX,NREC,NPNTMV,NPNTVL,NPNTD,NPDELC
     1,NPNCHV,PINT,TIMX,TINIT
      WRITE (6,1080) INT
      WRITE (6,1090) NTIM,NPNT,NITP,ITMAX,NREC,NPNTMV,NPNTVL,NPNTD,NPDEL
     1C,NPNCHV,PINT,TIMX,TINIT
C     ******************************************************************
C     ---LIST TIME INCREMENTS---
   20 DO 30 J=1,100
      TIM(J)=0.0
   30 CONTINUE
      TIM(1)=TINIT
      IF (S.EQ.0.0) GO TO 50
      DO 40 K=2,NTIM
   40 TIM(K)=TIMX*TIM(K-1)
      WRITE (6,470)
      WRITE (6,490) TIM
      GO TO 60
   50 TIM(1)=PYR
      WRITE (6,480) TIM(1)
C     ******************************************************************
C     ---INITIALIZE MATRICES---
   60 IF (INT.GT.1) GO TO 100
      DO 70 IY=1,NY
      DO 70 IX=1,NX
      VPRM(IX,IY)=0.0
      PERM(IX,IY)=0.0
      THCK(IX,IY)=0.0
      RECH(IX,IY)=0.0
      CNRECH(IX,IY)=0.0
      REC(IX,IY)=0.0
      NODEID(IX,IY)=0
      TMRX(IX,IY,1)=0.0
      TMRX(IX,IY,2)=0.0
      HI(IX,IY)=0.0
      HR(IX,IY)=0.0
      HC(IX,IY)=0.C
      HK(IX,IY)=0.0
      WT(IX,IY)=0.0
      VX(IX,IY)=0.0
```

FORTRAN IV program listing—Continued

```
      VY(IX,IY)=0.0
      VXBDY(IX,IY)=0.0
      VYBDY(IX,IY)=0.0
      CONC(IX,IY)=0.0
      CONINT(IX,IY)=0.0
      SUMC(IX,IY)=0.0
   70 CONTINUE
C     *****************************************************************
C     ---READ OBSERVATION WELL LOCATIONS---
      IF (NUMOBS.LE.0) GO TO 100
      WRITE (6,900)
      DO 80 J=1,NUMOBS
      READ (5,700) IX,IY
      WRITE (6,810) J,IX,IY
      IXOBS(J)=IX
   80 IYOBS(J)=IY
      DO 90 I=1,NUMOBS
      DO 90 J=1,50
      TMWL(I,J)=0.0
   90 TMCN(I,J)=0.0
C     *****************************************************************
C     ---READ PUMPAGE DATA -- (X-Y COORDINATES AND RATE IN CFS)---
C        ---SIGNS : WITHDRAWAL = POS.;  INJECTION = NEG.---
C        ---IF INJ. WELL, ALSO READ CONCENTRATION OF INJECTED WATER---
  100 IF (NREC.LE.0) GO TO 120
      WRITE (6,910)
      DO 110 I=1,NREC
      READ (5,710) IX,IY,FCTR,CNREC
      IF (FCTR.LT.0.0) CNRECH(IX,IY)=CNREC
      REC(IX,IY)=FCTR
  110 WRITE (6,820) IX,IY,REC(IX,IY),CNRECH(IX,IY)
C     *****************************************************************
  120 IF (INT.GT.1) RETURN
      AREA=XDEL*YDEL
      WRITE (6,690) AREA
      WRITE (6,600)
      WRITE (6,610) XDEL
      WRITE (6,610) YDEL
C     *****************************************************************
C     ---READ TRANSMISSIVITY IN FT**2/SEC INTO VPRM ARRAY---
C        ---FCTR = TRANSMISSIVITY MULTIPLIER  ---> FT**2/SEC---
      WRITE (6,530)
      READ (5,550) INPUT,FCTR
      DO 160 IY=1,NY
      IF (INPUT.EQ.1) READ (5,560) (VPRM(IX,IY),IX=1,NX)
      DO 150 IX=1,NX
      IF (INPUT.NE.1) GO TO 130
      VPRM(IX,IY)=VPRM(IX,IY)*FCTR
      GO TO 140
  130 VPRM(IX,IY)=FCTR
  140 IF (IX.EQ.1.OR.IX.EQ.NX) VPRM(IX,IY)=0.0
      IF (IY.EQ.1.OR.IY.EQ.NY) VPRM(IX,IY)=0.0
  150 CONTINUE
  160 WRITE (6,520) (VPRM(IX,IY),IX=1,NX)
C     *****************************************************************
C     ---SET UP COEFFICIENT MATRIX --- BLOCK-CENTERED GRID---
C     ---AVERAGE TRANSMISSIVITY --- HARMONIC MEAN---
      IF (ANFCTR.NE.0.0) GO TO 170
      WRITE (6,1050)
      ANFCTR=1.0
  170 PIES=3.1415927*3.1415927/2.0
      YNS=NY*NY
```

FORTRAN IV program listing—Continued

```
      XNS=NX*NX
      HMIN=2.0
      DO 180 IY=2,NNY
      DO 180 IX=2,NNX
      IF (VPRM(IX,IY).EQ.0.0) GO TO 180
      TMRX(IX,IY,1)=2.0*VPRM(IX,IY)*VPRM(IX+1,IY)/(VPRM(IX,IY)*XDEL+VPRM
     1(IX+1,IY)*XDEL)
      TMRX(IX,IY,2)=2.0*VPRM(IX,IY)*VPRM(IX,IY+1)/(VPRM(IX,IY)*YDEL+VPRM
     1(IX,IY+1)*YDEL)
C         ---ADJUST COEFFICIENT FOR ANISOTROPY---
      TMRX(IX,IY,2)=TMRX(IX,IY,2)*ANFCTR
C         ---COMPUTE MINIMUM ITERATION PARAMETER (HMIN)---
      IF (TMRX(IX,IY,1).EQ.0.0) GO TO 180
      IF (TMRX(IX,IY,2).EQ.0.0) GO TO 180
      RAT=TMRX(IX,IY,1)*YDEL/(TMRX(IX,IY,2)*XDEL)
      HMX=PIES/(XNS*(1.0+RAT))
      HMY=PIES/(YNS*(1.0+(1.0/RAT)))
      IF (HMX.LT.HMIN) HMIN=HMX
      IF (HMY.LT.HMIN) HMIN=HMY
  180 CONTINUE
C     *****************************************************************
C     ---READ AQUIFER THICKNESS---
      WRITE (6,510)
      READ (5,550) INPUT,FCTR
      DO 210 IY=1,NY
      IF (INPUT.EQ.1) READ (5,540) (THCK(IX,IY),IX=1,NX)
      DO 200 IX=1,NX
      IF (INPUT.NE.1) GO TO 190
      THCK(IX,IY)=THCK(IX,IY)*FCTR
      GO TO 200
  190 IF (VPRM(IX,IY).NE.0.0) THCK(IX,IY)=FCTR
  200 CONTINUE
  210 WRITE (6,500) (THCK(IX,IY),IX=1,NX)
C     *****************************************************************
C     ---READ DIFFUSE RECHARGE AND DISCHARGE---
      WRITE (6,830)
      READ (5,550) INPUT,FCTR
      DO 240 IY=1,NY
      IF (INPUT.EQ.1) READ (5,560) (RECH(IX,IY),IX=1,NX)
      DO 230 IX=1,NX
      IF (INPUT.NE.1) GO TO 220
      RECH(IX,IY)=RECH(IX,IY)*FCTR
      GO TO 230
  220 IF (THCK(IX,IY).NE.0.0) RECH(IX,IY)=FCTR
  230 CONTINUE
  240 WRITE (6,840) (RECH(IX,IY),IX=1,NX)
C     *****************************************************************
C     ---COMPUTE PERMEABILITY FROM TRANSMISSIVITY---
C     ---COUNT NO. OF CELLS IN AQUIFER---
C     ---SET NZCRIT = 2% OF THE NO. OF CELLS IN THE AQUIFER---
      DO 250 IX=1,NX
      DO 250 IY=1,NY
      IF (THCK(IX,IY).EQ.0.0) GO TO 250
      PERM(IX,IY)=VPRM(IX,IY)/THCK(IX,IY)
      NCA=NCA+1
  250 VPRM(IX,IY)=0.0
C
      AAQ=NCA*AREA
      NZCRIT=(NCA+25)/50
      WRITE (6,620)
      DO 260 IY=1,NY
  260 WRITE (6,650) (PERM(IX,IY),IX=1,NX)
```

FORTRAN IV program listing—Continued

```
      WRITE (6,630) NCA,AAQ,NZCRIT
C     ******************************************************************
C     ---READ NODE IDENTIFICATION CARDS---
C        ---SET VERT. PERM., SOURCE CONC., AND DIFFUSE RECHARGE---
C           ---SPECIFY CODES TO FIT YOUR NEEDS---
      WRITE (6,570)
      READ (5,550) INPUT,FCTR
      DO 280 IY=1,NY
      IF (INPUT.EQ.1) READ (5,640) (NODEID(IX,IY),IX=1,NX)
      DO 270 IX=1,NX
  270 IF (INPUT.NE.1.AND.THCK(IX,IY).NE.0.0) NODEID(IX,IY)=FCTR
  280 WRITE (6,580) (NODEID(IX,IY),IX=1,NX)
      WRITE (6,920) NCODES
      IF (NCODES.LE.0) GO TO 310
      WRITE (6,930)
      DO 300 IJ=1,NCODES
      READ (5,850) ICODE,FCTR1,FCTR2,FCTR3,OVERRD
      DO 290 IX=1,NX
      DO 290 IY=1,NY
      IF (NODEID(IX,IY).NE.ICODE) GO TO 290
      VPRM(IX,IY)=FCTR1
      CNRECH(IX,IY)=FCTR2
      IF (OVERRD.NE.0) RECH(IX,IY)=FCTR3
  290 CONTINUE
      WRITE (6,860) ICODE,FCTR1,FCTR2
  300 IF (OVERRD.NE.0) WRITE (6,1100) FCTR3
  310 WRITE (6,590)
      DO 320 IY=1,NY
  320 WRITE (6,520) (VPRM(IX,IY),IX=1,NX)
C     ******************************************************************
C     ---READ WATER-TABLE ELEVATION---
      WRITE (6,670)
      READ (5,550) INPUT,FCTR
      DO 350 IY=1,NY
      IF (INPUT.EQ.1) READ (5,660) (WT(IX,IY),IX=1,NX)
      DO 340 IX=1,NX
      IF (INPUT.NE.1) GO TO 330
      WT(IX,IY)=WT(IX,IY)*FCTR
      GO TO 340
  330 IF (THCK(IX,IY).NE.0.0) WT(IX,IY)=FCTR
  340 CONTINUE
  350 WRITE (6,680) (WT(IX,IY),IX=1,NX)
C     ******************************************************************
C     ---SET INITIAL HEADS---
      DO 360 IX=1,NX
      DO 360 IY=1,NY
      HI(IX,IY)=WT(IX,IY)
      HC(IX,IY)=HI(IX,IY)
      HR(IX,IY)=HI(IX,IY)
  360 HK(IX,IY)=HI(IX,IY)
C
      CALL OUTPT
C     ******************************************************************
C     ---COMPUTE ITERATION PARAMETERS---
      DO 370 ID=1,20
      AOPT(ID)=0.0
  370 CONTINUE
      ANITP=NITP-1
      ALPHA1=DEXP(DLOG(1.0/HMIN)/ANITP)
      AOPT(1)=HMIN
      DO 380 IP=2,NITP
  380 AOPT(IP)=AOPT(IP-1)*ALPHA1
```

FORTRAN IV program listing—Continued

```
C
      WRITE (6,450)
      WRITE (6,460) AOPT
C     ****************************************************************
C     ---READ INITIAL CONCENTRATIONS AND COMPUTE INITIAL MASS STORED---
      READ (5,550) INPUT,FCTR
      DO 420 IY=1,NY
      IF (INPUT.EQ.1) READ (5,660) (CONC(IX,IY),IX=1,NX)
      DO 410 IX=1,NX
      IF (INPUT.NE.1) GO TO 390
      CONC(IX,IY)=CONC(IX,IY)*FCTR
      GO TO 400
  390 IF (THCK(IX,IY).NE.0.0) CONC(IX,IY)=FCTR
  400 CONINT(IX,IY)=CONC(IX,IY)
  410 STORMI=STORMI+CONINT(IX,IY)*THCK(IX,IY)*AREA*POROS
  420 CONTINUE
C     ****************************************************************
C     ---CHECK DATA SETS FOR INTERNAL CONSISTENCY---
      DO 440 IX=1,NX
      DO 440 IY=1,NY
      IF (THCK(IX,IY).GT.0.0) GO TO 430
      IF (TMRX(IX,IY,1).GT.0.0) WRITE (6,940) IX,IY
      IF (TMRX(IX,IY,2).GT.0.0) WRITE (6,950) IX,IY
      IF (NODEID(IX,IY).GT.0) WRITE (6,960) IX,IY
      IF (WT(IX,IY).NE.0.0) WRITE (6,970) IX,IY
      IF (RECH(IX,IY).NE.0.0) WRITE (6,980) IX,IY
      IF (REC(IX,IY).NE.0.0) WRITE (6,990) IX,IY
  430 IF (PERM(IX,IY).GT.0.0) GO TO 440
      IF (NODEID(IX,IY).GT.0.0) WRITE (6,1000) IX,IY
      IF (WT(IX,IY).NE.0.0) WRITE (6,1010) IX,IY
      IF (RECH(IX,IY).NE.0.0) WRITE (6,1020) IX,IY
      IF (REC(IX,IY).NE.0.0) WRITE (6,1030) IX,IY
      IF (THCK(IX,IY).GT.0.0) WRITE (6,1040) IX,IY
  440 CONTINUE
C     ****************************************************************
      RETURN
C     ****************************************************************
C
C
C
  450 FORMAT (1H1,20HITERATION PARAMETERS)
  460 FORMAT (3H    ,1G20.6)
  470 FORMAT (1H1,27HTIME INTERVALS (IN SECONDS))
  480 FORMAT (1H1,15X,17HSTEADY-STATE FLOW//5X,57HTIME INTERVAL (IN SEC)
     1 FOR SOLUTE-TRANSPORT SIMULATION = ,G12.5)
  490 FORMAT (3H    ,10G12.5)
  500 FORMAT (3H    ,20F5.1)
  510 FORMAT (1H1,22HAQUIFER THICKNESS (FT))
  520 FORMAT (3H    ,20F5.2)
  530 FORMAT (1H1,30HTRANSMISSIVITY MAP (FT*FT/SEC))
  540 FORMAT (20G3.0)
  550 FORMAT (I1,G10.0)
  560 FORMAT (20G4.1)
  570 FORMAT (1H1,23HNODE IDENTIFICATION MAP//)
  580 FORMAT (1H ,20I5)
  590 FORMAT (1H1,45HVERTICAL PERMEABILITY/THICKNESS (FT/(FT*SEC)))
  600 FORMAT (1H0,10X,12HX-Y SPACING:)
  610 FORMAT (1H ,12X,10G12.5)
  620 FORMAT (1H1,24HPERMEABILTY MAP (FT/SEC))
  630 FORMAT (1H0,////10X,44HNO. OF FINITE-DIFFERENCE CELLS IN AQUIFER =
     1 ,I4//10X,28HAREA OF AQUIFER IN MODEL  = ,G12.5,10H   SQ. FT.////1
     20X,47HNZCRIT   (MAX. NO. OF CELLS THAT CAN BE VOID OF/20X,56HPARTI
```

FORTRAN IV program listing—Continued

```
   3CLES;  IF EXCEEDED, PARTICLES ARE REGENERATED)   = ,I4/)
  640 FORMAT (20I1)
  650 FORMAT (3H    ,20F5.3)
  660 FORMAT (20G4.0)
  670 FORMAT (1H1,11HWATER TABLE)
  680 FORMAT (1H ,20F5.0)
  690 FORMAT (1H0,10X,19HAREA OF ONE CELL = ,G12.4)
  700 FORMAT (2I2)
  710 FORMAT (2I2,2G8.2)
  720 FORMAT (10A8)
  730 FORMAT (1H0,10A8)
  740 FORMAT (17I4)
  750 FORMAT (1H1,77HU.S.G.S. METHOD-OF-CHARACTERISTICS MODEL FOR SOLUTE
     1 TRANSPORT IN GROUND WATER)
  760 FORMAT (1H0,21X,21HI N P U T     D A T A)
  770 FORMAT (1H0,23X,16HGRID DESCRIPTORS//13X,30HNX    (NUMBER OF COLUM
     1NS)  =   ,I4/13X,28HNY    (NUMBER OF ROWS)     =,I6/13X,29HXDEL  (X
     2-DISTANCE IN FEET) = ,F7.1/13X,29HYDEL  (Y-DISTANCE IN FEET) = ,F7
     3.1)
  780 FORMAT (1H0,23X,16HTIME  PARAMETERS//13X,40HNTIM   (MAX. NO. OF TI
     1ME STEPS)        = ,I6/13X,40HNPMP   (NO. OF PUMPING PERIODS)
     2 = ,I6/13X,39HPINT   (PUMPING PERIOD IN YEARS)       =,F10.2/13X,39
     3HTIMX    (TIME INCREMENT MULTIPLIER)    =,F10.2/13X,39HTINIT  (INIT
     4IAL TIME STEP IN SEC.)     =,F8.0)
  790 FORMAT (1H0,14X,34HHYDROLOGIC AND CHEMICAL PARAMETERS//13X,1HS,7X,
     129H(STORAGE COEFFICIENT)        =,5X,F9.6/13X,28HPOROS   (EFFECTIVE
     2 POROSITY),8X,3H=  ,F8.2/13X,39HBETA    (CHARACTERISTIC LENGTH)
     3  =  ,F7.1/13X,31HDLTRAT  (RATIO OF TRANSVERSE TO/21X,30HLONGITUDI
     4NAL DISPERSIVITY)  = ,F9.2/13X,39HANFCTR  (RATIO OF T-YY TO T-XX)
     5    =   ,F12.6)
  800 FORMAT (12G5.0)
  810 FORMAT (1H ,16X,I2,5X,I2,4X,I2)
  820 FORMAT (1H ,7X,2I4,3X,F7.2,5X,F7.1)
  830 FORMAT (1H1,39HDIFFUSE RECHARGE AND DISCHARGE (FT/SEC))
  840 FORMAT (1H ,1P10E10.2)
  850 FORMAT (I2,3G10.2,I2)
  860 FORMAT (1H0,7X,I2,7X,E10.3,5X,F9.2)
  870 FORMAT (1H0,21X,20HEXECUTION PARAMETERS//13X,39HNITP   (NO. OF ITE
     1RATION PARAMETERS) = ,I4/13X,39HTOL    (CONVERGENCE CRITERIA - ADI
     2P) = ,F9.4/13X,39HITMAX  (MAX.NO.OF ITERATIONS - ADIP) = ,I4/13X,3
     34HCELDIS (MAX.CELL DISTANCE PER MOVE/24X,28HOF PARTICLES - M.O.C.)
     4    = ,F8.3/13X,30HNPMAX  (MAX. NO. OF PARTICLES),7X,2H= ,I4/12X,3
     52H NPTPND (NO. PARTICLES PER NODE),6X,3H=  ,I4)
  880 FORMAT (1H0,5X,47H*** WARNING ***  NPTPND MUST EQUAL 4,5,8, OR 9.)
  890 FORMAT (1H0,23X,15HPROGRAM OPTIONS//13X,30HNPNT    (TIME STEP INTER
     1VAL FOR/21X,18HCOMPLETE PRINTOUT),7X,3H=  ,I4/13X,31HNPNTMV (MOVE
     2INTERVAL FOR CHEM./21X,28HCONCENTRATION PRINTOUT)  =   ,I4/13X,29HN
     3PNTVL (PRINT OPTION-VELOCITY/21X,24H0=NO; 1=FIRST TIME STEP;/21X,1
     47H2=ALL TIME STEPS),8X,3H=  ,I4/13X,31HNPNTD  (PRINT OPTION-DISP.C
     5OEF./21X,24H0=NO; 1=FIRST TIME STEP;/21X,17H2=ALL TIME STEPS),8X,3
     6H=  ,I4/13X,32HNUMOBS (NO. OF OBSERVATION WELLS/21X,28HFOR HYDROGR
     7APH PRINTOUT) =  ,I4/13X,35HNREC   (NO. OF PUMPING WELLS)    = ,I5
     8/13X,24HNCODES (FOR NODE IDENT.),9X,2H= ,I5/13X,25HNPNCHV (PUNCH V
     9ELOCITIES),8X,2H= ,I5/13X,36HNPDELC (PRINT OPT.-CONC. CHANGE) =  ,
     $I4)
  900 FORMAT (1H0,10X,29HLOCATION OF OBSERVATION WELLS//17X,3HNO.,5X,1HX
     1,5X,1HY/)
  910 FORMAT (1H0,10X,28HLOCATION   OF   PUMPING   WELLS//11X,28HX    Y    RA
     1TE(IN CFS)    CONC./)
  920 FORMAT (1H0,5X,37HNO. OF NODE IDENT. CODES SPECIFIED = ,I2)
  930 FORMAT (1H0,10X,41HTHE FOLLOWING ASSIGNMENTS HAVE BEEN MADE:/5X,51
     1HCODE NO.     LEAKANCE      SOURCE CONC.      RECHARGE)
```

FORTRAN IV program listing—Continued

```
  940 FORMAT (1H ,5X,61H*** WARNING ***   THCK.EQ.0.0 AND TMRX(X).GT.0.0
     1 AT NODE IX =,I4,6H, IY =,I4)
  950 FORMAT (1H ,5X,61H*** WARNING ***   THCK.EQ.0.0 AND TMRX(Y).GT.0.0
     1 AT NODE IX =,I4,6H, IY =,I4)
  960 FORMAT (1H ,5X,61H*** WARNING ***    THCK.EQ.0.0 AND NODEID.GT.0.0
     1 AT NODE IX =,I4,6H, IY =,I4)
  970 FORMAT (1H ,5X,56H*** WARNING ***   THCK.EQ.0.0 AND WT.NE.0.0 AT N
     1ODE IX =,I4,6H, IY =,I4)
  980 FORMAT (1H ,5X,58H*** WARNING ***   THCK.EQ.0.0 AND RECH.NE.0.0 AT
     1 NODE IX =,I4,6H, IY =,I4)
  990 FORMAT (1H ,5X,58H*** WARNING ***    THCK.EQ.0.0 AND REC.NE.0.0 AT
     1 NODE IX =,I4,6H, IY =,I4)
 1000 FORMAT (1H ,5X,61H*** WARNING ***    PERM.EQ.0.0 AND NODEID.GT.0.0
     1 AT NODE IX =,I4,6H, IY =,I4)
 1010 FORMAT (1H ,5X,56H*** WARNING ***   PERM.EQ.0.0 AND WT.NE.0.0 AT N
     1ODE IX =,I4,6H, IY =,I4)
 1020 FORMAT (1H ,5X,58H*** WARNING ***   PERM.EQ.0.0 AND RECH.NE.0.0 AT
     1 NODE IX =,I4,6H, IY =,I4)
 1030 FORMAT (1H ,5X,58H*** WARNING ***    PERM.EQ.0.0 AND REC.NE.0.0 AT
     1 NODE IX =,I4,6H, IY =,I4)
 1040 FORMAT (1H ,5X,58H*** WARNING ***   PERM.EQ.0.0 AND THCK.GT.0.0 AT
     1 NODE IX =,I4,6H, IY =,I4)
 1050 FORMAT (1H0,5X,45H*** WARNING ***   ANFCTR WAS SPECIFIED AS 0.0/23
     1X,34HDEFAULT ACTION: RESET ANFCTR = 1.0)
 1060 FORMAT (I1)
 1070 FORMAT (10I4,3G5.0)
 1080 FORMAT (1H1,5X,25HSTART PUMPING PERIOD NO. ,I2//2X,75HTHE FOLLOWIN
     1G TIME STEP, PUMPAGE, AND PRINT PARAMETERS HAVE BEEN REDEFINED:/)
 1090 FORMAT (1HC,14X,9HNTIM     = ,I4/15X,9HNPNT     = ,I4/15X,9HNITP     = ,
     1I4/15X,9HITMAX    = ,I4/15X,9HNREC     = ,I4/15X,9HNPNTMV = ,I4/15X,9H
     2NPNTVL = ,I4/15X,9HNPNTD  = ,I4/15X,9HNPDELC = ,I4/15X,9HNPNCHV =
     3,I4/15X,9HPINT    = ,F10.3/15X,9HTIMX     = ,F10.3/15X,9HTINIT   = ,F1
     40.3/)
 1100 FORMAT (1H ,46X,E10.3)
      END
      SUBROUTINE ITERAT
      DOUBLE PRECISION DMIN1,DEXP,DLOG,DABS
      REAL *8TMRX,VPRM,HI,HR,HC,HK,WT,REC,RECH,TIM,AOPT,TITLE
      REAL *8XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      REAL *8B,G,W,A,C,E,F,DR,DC,TBAR,TMK,COEF,BLH,BRK,CHK,QL,BRH
      COMMON /PRMI/ NTIM,NPMP,NPNT,NITP,N,NX,NY,NP,NREC,INT,NNX,NNY,NUMO
     1BS,NMOV,IMOV,NPMAX,ITMAX,NZCRIT,IPRNT,NPTPND,NPNTMV,NPNTVL,NPNTD,N
     2PNCHV,NPDELC
      COMMON /PRMK/ NODEID(20,20),NPCELL(20,20),LIMBO(500),IXOBS(5),IYOB
     1S(5)
      COMMON /HEDA/ THCK(20,20),PERM(20,20),TMWL(5,50),TMOBS(50),ANFCTR
      COMMON /HEDB/ TMRX(20,20,2),VPRM(20,20),HI(20,20),HR(20,20),HC(20,
     120),HK(20,20),WT(20,20),REC(20,20),RECH(20,20),TIM(100),AOPT(20),T
     2ITLE(10),XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /BALM/ TOTLQ
      COMMON /XINV/ DXINV,DYINV,ARINV,PORINV
      DIMENSION W(20), B(20), G(20)
C     ****************************************************************
      KOUNT=0
C     ---COMPUTE ROW AND COLUMN---
C        ---CALL NEW ITERATION PARAMETER---
   10 REMN=MOD(KOUNT,NITP)
      IF (REMN.EQ.0) NTH=0
      NTH=NTH+1
      PARAM=AOPT(NTH)
C     ****************************************************************
C     ---ROW COMPUTATIONS---
```

FORTRAN IV program listing—Continued

```
      TEST=0.0
      RHO=S/TIM(N)
      BRK=-RHO
      DO 50 IY=1,NY
      DO 20 M=1,NX
      W(M)=0.0
      B(M)=0.0
      G(M)=0.0
   20 CONTINUE
      DO 30 IX=1,NX
      IF (THCK(IX,IY).EQ.0.0) GO TO 30
      COEF=VPRM(IX,IY)
      QL=-COEF*WT(IX,IY)
      A=TMRX(IX-1,IY,1)*DXINV
      C=TMRX(IX,IY,1)*DXINV
      E=TMRX(IX,IY-1,2)*DYINV
      F=TMRX(IX,IY,2)*DYINV
      TBAR=A+C+E+F
      TMK=TBAR*PARAM
      BLH=-A-C-RHO-COEF-TMK
      BRH=E+F-TMK
      DR=BRH*HC(IX,IY)+BRK*HK(IX,IY)-E*HC(IX,IY-1)-F*HC(IX,IY+1)+QL+RECH
     1(IX,IY)+REC(IX,IY)*ARINV
      W(IX)=BLH-A*B(IX-1)
      B(IX)=C/W(IX)
      G(IX)=(DR-A*G(IX-1))/W(IX)
   30 CONTINUE
C
C         ---BACK SUBSTITUTION---
      DO 40 J=2,NX
      IJ=J-1
      IS=NX-IJ
   40 HR(IS,IY)=G(IS)-B(IS)*HR(IS+1,IY)
   50 CONTINUE
C     ****************************************************************
C     ---COLUMN COMPUTATIONS---
      DO 90 IX=1,NX
      DO 60 M=1,NY
      W(M)=0.0
      B(M)=0.0
   60 G(M)=0.0
      DO 70 IY=1,NY
      IF (THCK(IX,IY).EQ.0.0) GO TO 70
      COEF=VPRM(IX,IY)
      QL=-COEF*WT(IX,IY)
      A=TMRX(IX,IY-1,2)*DYINV
      C=TMRX(IX,IY,2)*DYINV
      E=TMRX(IX-1,IY,1)*DXINV
      F=TMRX(IX,IY,1)*DXINV
      TBAR=A+C+E+F
      TMK=TBAR*PARAM
      BLH=-A-C-RHO-COEF-TMK
      BRH=E+F-TMK
      DC=BRH*HR(IX,IY)+BRK*HK(IX,IY)-E*HR(IX-1,IY)-F*HR(IX+1,IY)+QL+RECH
     1(IX,IY)+REC(IX,IY)*ARINV
      W(IY)=BLH-A*B(IY-1)
      B(IY)=C/W(IY)
      G(IY)=(DC-A*G(IY-1))/W(IY)
   70 CONTINUE
C
C         ---BACK SUBSTITUTION---
      DO 80 J=2,NY
```

FORTRAN IV program listing—Continued

```
      IJ=J-1
      IB=NY-IJ
      HC(IX,IB)=G(IB)-B(IB)*HC(IX,IB+1)
      IF (THCK(IX,IB).EQ.0.0) GO TO 80
      CHK=DABS(HC(IX,IB)-HR(IX,IB))
      IF (CHK.GT.TOL) TEST=1.0
   80 CONTINUE
   90 CONTINUE
C     ****************************************************************
      KOUNT=KOUNT+1
      IF (TEST.EQ.0.0) GO TO 120
      IF (KOUNT.GE.ITMAX) GO TO 100
      GO TO 10
C     *****************************************************************
C     ---TERMINATE PROGRAM -- ITMAX EXCEEDED---
  100 WRITE (6,160)
      DO 110 IX=1,NX
      DO 110 IY=1,NY
  110 HK(IX,IY)=HC(IX,IY)
      CALL OUTPT
      STOP
C     *****************************************************************
C     ---SET NEW HEAD (HK)---
  120 DO 130 IY=1,NY
      DO 130 IX=1,NX
      IF (THCK(IX,IY).EQ.0.0) GO TO 130
      HR(IX,IY)=HK(IX,IY)
      HK(IX,IY)=HC(IX,IY)
C
C     ---COMPUTE LEAKAGE FOR MASS BALANCE---
      IF (VPRM(IX,IY).EQ.0.0) GO TO 130
      DELQ=VPRM(IX,IY)*AREA*(WT(IX,IY)-HK(IX,IY))
      TOTLQ=TOTLQ+DELQ*TIM(N)
  130 CONTINUE
C
      WRITE (6,140) N
      WRITE (6,150) KOUNT
C     *****************************************************************
      RETURN
C     *****************************************************************
C
C
C
  140 FORMAT (1HC//3X,4HN = ,1I4)
  150 FORMAT (1H ,2X,23HNUMBER OF ITERATIONS = ,1I4)
  160 FORMAT (1H0,5X,64H***   EXECUTION TERMINATED -- MAX. NO. ITERATION
     1S EXCEEDED   ***/26X,21HFINAL OUTPUT FOLLOWS:)
      END
      SUBROUTINE GENPT
      REAL *8TMRX,VPRM,HI,HR,HC,HK,WT,REC,RECH,TIM,AOPT,TITLE
      REAL *8XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /PRMI/ NTIM,NPMP,NPNT,NITP,N,NX,NY,NP,NREC,INT,NNX,NNY,NUMO
     1BS,NMOV,IMOV,NPMAX,ITMAX,NZCRIT,IPRNT,NPTPND,NPNTMV,NPNTVL,NPNTD,N
     2PNCHV,NPDELC
      COMMON /PRMK/ NODEID(20,20),NPCELL(20,20),LIMBO(500),IXOBS(5),IYOB
     1S(5)
      COMMON /HEDA/ THCK(20,20),PERM(20,20),TMWL(5,50),TMOBS(50),ANFCTR
      COMMON /HEDB/ TMRX(20,20,2),VPRM(20,20),HI(20,20),HR(20,20),HC(20,
     120),HK(20,20),WT(20,20),REC(20,20),RECH(20,20),TIM(100),AOPT(20),T
     2ITLE(10),XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /CHMA/ PART(3,3200),CONC(20,20),TMCN(5,50),VX(20,20),VY(20,
     120),CONINT(20,20),CNRECH(20,20),POROS,SUMTCH,BETA,TIMV,STORM,STORM
```

FORTRAN IV program listing—Continued

```
     2I,CMSIN,CMSOUT,FLMIN,FLMOT,SUMIO,CELDIS,DLTRAT,CSTORM
      DIMENSION RP(8), RN(8), IPT(8)
C     ******************************************************************
      F1=0.30
      F2=1.0/3.0
      IF (NPTPND.EQ.4) F1=0.25
      IF (NPTPND.EQ.9) F1=1.0/3.0
      IF (NPTPND.EQ.8) F2=0.25
      NCHK=NPTPND
      IF (NPTPND.EQ.5.OR.NPTPND.EQ.9) NCHK=NPTPND-1
      IF (TEST.GT.98.) GO TO 10
C     ******************************************************************
C     ---INITIALIZE VALUES---
      STORM=0.0
      CMSIN=0.0
      CMSOUT=0.0
      FLMIN=0.0
      FLMOT=0.0
      SUMIO=0.0
C     ******************************************************************
   10 DO 20 ID=1,3
      DO 20 IN=1,NPMAX
   20 PART(ID,IN)=0.0
      DO 30 IA=1,8
      RP(IA)=0.0
      RN(IA)=0.0
   30 IPT(IA)=0
C     ---SET UP LIMBO ARRAY---
      DO 40 IN=1,500
   40 LIMBO(IN)=0.0
      IND=1
      DO 50 IL=1,500,2
      LIMBO(IL)=IND
   50 IND=IND+1
C     ******************************************************************
C     ---INSERT PARTICLES---
      DO 410 IX=1,NX
      DO 410 IY=1,NY
      IF (THCK(IX,IY).EQ.0.0) GO TO 410
      KR=0
      TEST2=0.0
      METH=1
      NPCELL(IX,IY)=0
      C1=CONC(IX,IY)
      IF (C1.LE.1.0E-05) TEST2=1.0
      IF (VPRM(IX,IY).GT.0.09) TEST2=1.0
      IF (REC(IX,IY).NE.0.0) TEST2=1.0
      IF (THCK(IX+1,IY+1).EQ.0.0.OR.THCK(IX+1,IY-1).EQ.0.0.OR.THCK(IX-1,
     1IY+1).EQ.0.0.OR.THCK(IX-1,IY-1).EQ.0.0) TEST2=1.0
      IF ((THCK(IX,IY+1).EQ.0.0.OR.THCK(IX,IY-1).EQ.0.0.OR.THCK(IX+1,IY)
     1.EQ.0.0.OR.THCK(IX-1,IY).EQ.0.0).AND.NPTPND.GT.5) TEST2=1.0
      CNODE=C1*(1.0-F1)
      IF (TEST.LT.98.0.OR.TEST2.GT.0.0) GO TO 70
      SUMC=CONC(IX+1,IY)+CONC(IX-1,IY)+CONC(IX,IY+1)+CONC(IX,IY-1)
      IF (NCHK.EQ.4) GO TO 60
      SUMC=SUMC+CONC(IX+1,IY+1)+CONC(IX+1,IY-1)+CONC(IX-1,IY+1)+CONC(IX-
     11,IY-1)
   60 AVC=SUMC/NCHK
      IF (AVC.GT.C1) METH=2
C
C        ---PUT 4 PARTICLES ON CELL DIAGONALS---
   70 DO 140 IT=1,2
```

FORTRAN IV program listing—Continued

```
      EVET=(-1.0)**IT
      DO 140 IS=1,2
      EVES=(-1.0)**IS
      PART(1,IND)=IX+F1*EVET
      PART(2,IND)=IY+F1*EVES
      PART(2,IND)=-PART(2,IND)
      PART(3,IND)=C1
      IF (TEST.LT.98.0.OR.TEST2.GT.0.0) GO TO 130
      IXD=IX+EVET
      IYD=IY+EVES
      KR=KR+1
      IPT(KR)=IND
      IF (METH.EQ.2) GO TO 80
      PART(3,IND)=CNODE+CONC(IXD,IYD)*F1
      GO TO 90
   80 PART(3,IND)=2.0*C1*CONC(IXD,IYD)/(C1+CONC(IXD,IYD))
   90 IF (C1-CONC(IXD,IYD)) 100,110,120
  100 RP(KR)=CONC(IXD,IYD)-PART(3,IND)
      RN(KR)=C1-PART(3,IND)
      GO TO 130
  110 RP(KR)=0.0
      RN(KR)=0.0
      GO TO 130
  120 RP(KR)=C1-PART(3,IND)
      RN(KR)=CONC(IXD,IYD)-PART(3,IND)
  130 IND=IND+1
  140 CONTINUE
C
      IF (NPTPND.EQ.5.OR.NPTPND.EQ.9) GO TO 150
      GO TO 160
C        ---PUT ONE PARTICLE AT CENTER OF CELL---
  150 PART(1,IND)=-IX
      PART(2,IND)=-IY
      PART(3,IND)=C1
      IND=IND+1
C        ---PLACE NORTH, SOUTH, EAST, AND WEST PARTICLES---
  160 IF (NPTPND.LT.8) GO TO 290
      CNODE=C1*(1.0-F2)
      DO 280 IT=1,2
      EVET=(-1.0)**IT
      PART(1,IND)=IX+F2*EVET
      PART(2,IND)=-IY
      PART(3,IND)=C1
      IF (TEST.LT.98.0.OR.TEST2.GT.0.0) GO TO 220
      IXD=IX+EVET
      KR=KR+1
      IPT(KR)=IND
      IF (METH.EQ.2) GO TO 170
      PART(3,IND)=CNODE+CONC(IXD,IY)*F2
      GO TO 180
  170 PART(3,IND)=2.0*C1*CONC(IXD,IY)/(C1+CONC(IXD,IY))
  180 IF (C1-CONC(IXD,IY)) 190,200,210
  190 RP(KR)=CONC(IXD,IY)-PART(3,IND)
      RN(KR)=C1-PART(3,IND)
      GO TO 220
  200 RP(KR)=0.0
      RN(KR)=0.0
      GO TO 220
  210 RP(KR)=C1-PART(3,IND)
      RN(KR)=CONC(IXD,IY)-PART(3,IND)
  220 IND=IND+1
      PART(1,IND)=IX
```

FORTRAN IV program listing—Continued

```
      PART(2,IND)=IY+F2*EVET
      PART(2,IND)=-PART(2,IND)
      PART(3,IND)=C1
      IF (TEST.LT.98.0.OR.TEST2.GT.0.0) GO TO 280
      IYD=IY+EVET
      KR=KR+1
      IPT(KR)=IND
      IF (METH.EQ.2) GO TO 230
      PART(3,IND)=CNODE+CONC(IX,IYD)*F2
      GO TO 240
  230 PART(3,IND)=2.0*C1*CONC(IX,IYD)/(C1+CONC(IX,IYD))
  240 IF (C1-CONC(IX,IYD)) 250,260,270
  250 RP(KR)=CONC(IX,IYD)-PART(3,IND)
      RN(KR)=C1-PART(3,IND)
      GO TO 280
  260 RP(KR)=0.0
      RN(KR)=0.0
      GO TO 280
  270 RP(KR)=C1-PART(3,IND)
      RN(KR)=CONC(IX,IYD)-PART(3,IND)
  280 IND=IND+1
C
  290 IF (TEST.LT.98.0.OR.TEST2.GT.0.0) GO TO 410
      SUMPT=0.0
C        ---COMPUTE CONC. GRADIENT WITHIN CELL---
      DO 300 KPT=1,NCHK
      IK=IPT(KPT)
  300 SUMPT=PART(3,IK)+SUMPT
      CBAR=SUMPT/NCHK
C        ---CHECK MASS BALANCE WITHIN CELL AND ADJUST PT. CONCS.---
      SUMPT=0.0
      IF (CBAR-C1) 310,410,330
  310 CRCT=1.0-(CBAR/C1)
      IF (METH.EQ.1) CRCT=CBAR/C1
      DO 320 KPT=1,NCHK
      IK=IPT(KPT)
      PART(3,IK)=PART(3,IK)+RP(KPT)*CRCT
  320 SUMPT=SUMPT+PART(3,IK)
      CBARN=SUMPT/NCHK
      GO TO 350
  330 CRCT=1.0-(C1/CBAR)
      IF (METH.EQ.1) CRCT=C1/CBAR
      DO 340 KPT=1,NCHK
      IK=IPT(KPT)
      PART(3,IK)=PART(3,IK)+RN(KPT)*CRCT
  340 SUMPT=SUMPT+PART(3,IK)
      CBARN=SUMPT/NCHK
  350 IF (CBARN.EQ.C1) GO TO 410
C        ---CORRECT FOR OVERCOMPENSATION---
      CRCT=C1/CBARN
      DO 380 KPT=1,NCHK
      IK=IPT(KPT)
      PART(3,IK)=PART(3,IK)*CRCT
C        ---CHECK CONSTRAINTS---
      IF (PART(3,IK)-C1) 360,380,370
  360 CLIM=C1-RP(KPT)+RN(KPT)
      IF (PART(3,IK).LT.CLIM) GO TO 390
      GO TO 380
  370 CLIM=C1+RP(KPT)-RN(KPT)
      IF (PART(3,IK).GT.CLIM) GO TO 390
  380 CONTINUE
      GO TO 410
```

FORTRAN IV program listing—Continued

```
  390 TEST2=1.0
      DO 400 KPT=1,NCHK
      IK=IPT(KPT)
  400 PART(3,IK)=C1
  410 CONTINUE
      NP=IND
      IF (INT.EQ.0) CALL CHMOT
C     ******************************************************************
      RETURN
C     ******************************************************************
      END
      SUBROUTINE VELO
      DOUBLE PRECISION DMIN1,DEXP,DLOG,DABS
      REAL *8TMRX,VPRM,HI,HR,HC,HK,WT,REC,RECH,TIM,AOPT,TITLE
      REAL *8XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      REAL *8RATE,SLEAK,DIV
      COMMON /PRMI/ NTIM,NPMP,NPNT,NITP,N,NX,NY,NP,NREC,INT,NNX,NNY,NUMO
     1BS,NMOV,IMCV,NPMAX,ITMAX,NZCRIT,IPRNT,NPTPND,NPNTMV,NPNTVL,NPNTD,N
     2PNCHV,NPDELC
      COMMON /PRMK/ NODEID(20,20),NPCELL(20,20),LIMBO(500),IXOBS(5),IYOB
     1S(5)
      COMMON /HEDA/ THCK(20,20),PERM(20,20),TMWL(5,50),TMOBS(50),ANFCTR
      COMMON /HEDB/ TMRX(20,20,2),VPRM(20,20),HI(20,20),HR(20,20),HC(20,
     120),HK(20,20),WT(20,20),REC(20,20),RECH(20,20),TIM(100),AOPT(20),T
     2ITLE(10),XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /XINV/ DXINV,DYINV,ARINV,PORINV
      COMMON /CHMA/ PART(3,3200),CONC(20,20),TMCN(5,50),VX(20,20),VY(20,
     120),CONINT(20,20),CNRECH(20,20),POROS,SUMTCH,BETA,TIMV,STORM,STORM
     2I,CMSIN,CMSOUT,FLMIN,FLMOT,SUMIO,CELDIS,DLTRAT,CSTORM
      COMMON /CHMC/ SUMC(20,20),VXBDY(20,20),VYBDY(20,20)
      COMMON /DIFUS/ DISP(20,20,4)
C     ******************************************************************
C     ---COMPUTE VELOCITIES AND STORE---
      VMAX=1.0E-10
      VMAY=1.0E-10
      VMXBD=1.0E-10
      VMYBD=1.0E-10
      TMV=TIM(N)
      LIM=0
C
      DO 20 IX=1,NX
      DO 20 IY=1,NY
      DO 10 IZ=1,4
   10 DISP(IX,IY,IZ)=0.0
C
      IF (THCK(IX,IY).EQ.0.0) GO TO 20
      RATE=REC(IX,IY)/AREA
      SLEAK=(HK(IX,IY)-WT(IX,IY))*VPRM(IX,IY)
      DIV=RATE+SLEAK+RECH(IX,IY)
C
C        ---VELOCITIES AT NODES---
C           ---X-DIRECTION---
      GRDX=(HK(IX-1,IY)-HK(IX+1,IY))*DXINV*0.50
      IF (THCK(IX-1,IY).EQ.0.0) GRDX=(HK(IX,IY)-HK(IX+1,IY))*DXINV
      IF (THCK(IX+1,IY).EQ.0.0) GRDX=(HK(IX-1,IY)-HK(IX,IY))*DXINV
      IF (THCK(IX-1,IY).EQ.0.0.AND.THCK(IX+1,IY).EQ.0.0) GRDX=0.0
      VX(IX,IY)=PERM(IX,IY)*GRDX*PORINV
      ABVX=ABS(VX(IX,IY))
      IF (ABVX.GT.VMAX) VMAX=ABVX
C           ---Y-DIRECTION---
      GRDY=(HK(IX,IY-1)-HK(IX,IY+1))*DYINV*0.50
      IF (THCK(IX,IY-1).EQ.0.0) GRDY=(HK(IX,IY)-HK(IX,IY+1))*DYINV
```

FORTRAN IV program listing—Continued

```
      IF (THCK(IX,IY+1).EQ.0.0) GRDY=(HK(IX,IY-1)-HK(IX,IY))*DYINV
      IF (THCK(IX,IY-1).EQ.0.0.AND.THCK(IX,IY+1).EQ.0.0) GRDY=0.0
      VY(IX,IY)=PERM(IX,IY)*GRDY*PORINV*ANFCTR
      ABVY=ABS(VY(IX,IY))
      IF (ABVY.GT.VMAY) VMAY=ABVY
C
C        ---VELOCITIES AT CELL BOUNDARIES---
      GRDX=(HK(IX,IY)-HK(IX+1,IY))*DXINV
      PERMX=2.0*PERM(IX,IY)*PERM(IX+1,IY)/(PERM(IX,IY)+PERM(IX+1,IY))
      VXBDY(IX,IY)=PERMX*GRDX*PORINV
      GRDY=(HK(IX,IY)-HK(IX,IY+1))*DYINV
      PERMY=2.0*PERM(IX,IY)*PERM(IX,IY+1)/(PERM(IX,IY)+PERM(IX,IY+1))
      VYBDY(IX,IY)=PERMY*GRDY*PORINV*ANFCTR
      ABVX=ABS(VXBDY(IX,IY))
      ABVY=ABS(VYBDY(IX,IY))
      IF (ABVX.GT.VMXBD) VMXBD=ABVX
      IF (ABVY.GT.VMYBD) VMYBD=ABVY
C
      IF (DIV.GE.0.0) GO TO 20
      TDIV=(POROS*THCK(IX,IY))/DABS(DIV)
      IF (TDIV.LT.TMV) TMV=TDIV
   20 CONTINUE
C     ****************************************************************
C     ---PRINT VELOCITIES---
      IF (NPNTVL.EQ.0) GO TO 80
      IF (NPNTVL.EQ.2) GO TO 30
      IF (NPNTVL.EQ.1.AND.N.EQ.1) GO TO 30
      GO TO 80
   30 WRITE (6,320)
      WRITE (6,330)
      DO 40 IY=1,NY
   40 WRITE (6,350) (VX(IX,IY),IX=1,NX)
      WRITE (6,340)
      DO 50 IY=1,NY
   50 WRITE (6,350) (VXBDY(IX,IY),IX=1,NX)
      WRITE (6,360)
      WRITE (6,330)
      DO 60 IY=1,NY
   60 WRITE (6,350) (VY(IX,IY),IX=1,NX)
      WRITE (6,340)
      DO 70 IY=1,NY
   70 WRITE (6,350) (VYBDY(IX,IY),IX=1,NX)
C     ---PUNCH VELOCITIES---
   80 IF (NPNCHV.EQ.0) GO TO 110
      IF (NPNCHV.EQ.2) GO TO 90
      IF (NPNCHV.EQ.1.AND.N.EQ.1) GO TO 90
      GO TO 110
   90 WRITE (7,510) NX,NY,XDEL,YDEL,VMAX,VMAY
      DO 100 IY=1,NY
      WRITE (7,520) (VX(IX,IY),IX=1,NX)
  100 WRITE (7,520) (VY(IX,IY),IX=1,NX)
C     *****************************************************************
C     ---COMPUTE NEXT TIME STEP---
  110 WRITE (6,390)
      WRITE (6,400) VMAX,VMAY
      WRITE (6,410) VMXBD,VMYBD
      TDELX=CELDIS*XDEL/VMAX
      TDELY=CELDIS*YDEL/VMAY
      TDELXB=CELDIS*XDEL/VMXBD
      TDELYB=CELDIS*YDEL/VMYBD
      TIMV=AMIN1(TDELX,TDELY,TDELXB,TDELYB)
      WRITE (6,310) TMV,TIMV
```

FORTRAN IV program listing—Continued

```
      IF (TMV.LT.TIMV) GO TO 120
      LIM=-1
      GO TO 130
  120 TIMV=TMV
      LIM=1
  130 NTIMV=TIM(N)/TIMV
      NMOV=NTIMV+1
      WRITE (6,420) TIMV,NTIMV,NMOV
      TIMV=TIM(N)/NMOV
      WRITE (6,370) TIM(N)
      WRITE (6,380) TIMV
C
      IF (BETA.EQ.0.0) GO TO 200
C     ****************************************************************
C     ---COMPUTE DISPERSION COEFFICIENTS---
      ALPHA=BETA
      ALNG=ALPHA
      TRAN=DLTRAT*ALPHA
      XX2=XDEL*XDEL
      YY2=YDEL*YDEL
      XY2=4.0*XDEL*YDEL
      DO 150 IX=2,NNX
      DO 150 IY=2,NNY
      IF (THCK(IX,IY).EQ.0.0) GO TO 150
      VXE=VXBDY(IX,IY)
      VYS=VYBDY(IX,IY)
      IF (THCK(IX+1,IY).EQ.0.0) GO TO 140
C        ---FORWARD COEFFICIENTS: X-DIRECTION---
      VYE=(VYBDY(IX,IY-1)+VYBDY(IX+1,IY-1)+VYS+VYBDY(IX+1,IY))/4.0
      VXE2=VXE*VXE
      VYE2=VYE*VYE
      VMGE=SQRT(VXE2+VYE2)
      IF (VMGE.LT.1.0E-20) GO TO 140
      DALN=ALNG*VMGE
      DTRN=TRAN*VMGE
      VMGE2=VMGE*VMGE
C           ---XX COEFFICIENT---
      DISP(IX,IY,1)=(DALN*VXE2+DTRN*VYE2)/(VMGE2*XX2)
C           ---XY COEFFICIENT---
      DISP(IX,IY,3)=(DALN-DTRN)*VXE*VYE/(VMGE2*XY2)
C        ---FORWARD COEFFICIENTS: Y-DIRECTION---
  140 IF (THCK(IX,IY+1).EQ.0.0) GO TO 150
      VXS=(VXBDY(IX-1,IY)+VXE+VXBDY(IX-1,IY+1)+VXBDY(IX,IY+1))/4.0
      VYS2=VYS*VYS
      VXS2=VXS*VXS
      VMGS=SQRT(VXS2+VYS2)
      IF (VMGS.LT.1.0E-20) GO TO 150
      DALN=ALNG*VMGS
      DTRN=TRAN*VMGS
      VMGS2=VMGS*VMGS
C           ---YY COEFFICIENT---
      DISP(IX,IY,2)=(DALN*VYS2+DTRN*VXS2)/(VMGS2*YY2)
C           ---YX COEFFICIENT---
      DISP(IX,IY,4)=(DALN-DTRN)*VXS*VYS/(VMGS2*XY2)
  150 CONTINUE
C     ****************************************************************
C     ---ADJUST CROSS-PRODUCT TERMS FOR ZERO THICKNESS---
      DO 160 IX=2,NNX
      DO 160 IY=2,NNY
      IF (THCK(IX,IY+1).EQ.0.0.OR.THCK(IX+1,IY+1).EQ.0.0.OR.THCK(IX,IY-1
     1).EQ.0.0.OR.THCK(IX+1,IY-1).EQ.0.0) DISP(IX,IY,3)=0.0
      IF (THCK(IX+1,IY).EQ.0.0.OR.THCK(IX+1,IY+1).EQ.0.0.OR.THCK(IX-1,IY
```

FORTRAN IV program listing—Continued

```
     1).EQ.0.0.OR.THCK(IX-1,IY+1).EQ.0.0) DISP(IX,IY,4)=0.0
  160 CONTINUE
C     ***************************************************************
C     ---CHECK FOR STABILITY OF EXPLICIT METHOD---
      TIMDIS=0.0
      DO 170 IX=2,NNX
      DO 170 IY=2,NNY
      TDCO=DISP(IX,IY,1)+DISP(IX,IY,2)
  170 IF (TDCO.GT.TIMDIS) TIMDIS=TDCO
      TIMDC=0.5/TIMDIS
      WRITE (6,440) TIMDC
      NTIMD=TIM(N)/TIMDC
      NDISP=NTIMD+1
      IF (NDISP.LE.NMOV) GO TO 180
      NMOV=NDISP
      TIMV=TIM(N)/NMOV
      LIM=0
  180 WRITE (6,430) TIMV,NTIMD,NMOV
C     ***************************************************************
C     ---ADJUST DISP. EQUATION COEFFICIENTS FOR SATURATED THICKNESS---
      DO 190 IX=2,NNX
      DO 190 IY=2,NNY
      BAVX=0.5*(THCK(IX,IY)+THCK(IX+1,IY))
      BAVY=0.5*(THCK(IX,IY)+THCK(IX,IY+1))
      DISP(IX,IY,1)=DISP(IX,IY,1)*BAVX
      DISP(IX,IY,2)=DISP(IX,IY,2)*BAVY
      DISP(IX,IY,3)=DISP(IX,IY,3)*BAVX
  190 DISP(IX,IY,4)=DISP(IX,IY,4)*BAVY
C     ***************************************************************
  200 IF (LIM) 210,220,230
  210 WRITE (6,530)
      GO TO 240
  220 WRITE (6,540)
      GO TO 240
  230 WRITE (6,550)
C     ***************************************************************
C     ---PRINT DISPERSION EQUATION COEFFICIENTS---
  240 IF (NPNTD.EQ.0) GO TO 300
      IF (NPNTD.EQ.2) GO TO 250
      IF (NPNTD.EQ.1.AND.N.EQ.1) GO TO 250
      GO TO 300
  250 WRITE (6,450)
      WRITE (6,460)
      DO 260 IY=1,NY
  260 WRITE (6,500) (DISP(IX,IY,1),IX=1,NX)
      WRITE (6,470)
      DO 270 IY=1,NY
  270 WRITE (6,500) (DISP(IX,IY,2),IX=1,NX)
      WRITE (6,480)
      DO 280 IY=1,NY
  280 WRITE (6,500) (DISP(IX,IY,3),IX=1,NX)
      WRITE (6,490)
      DO 290 IY=1,NY
  290 WRITE (6,500) (DISP(IX,IY,4),IX=1,NX)
C     ***************************************************************
  300 RETURN
C     ***************************************************************
C
C
C
  310 FORMAT (1H ,19H TMV (MAX. INJ.) = ,G12.5/20H  TIMV (CELDIS)   = ,G
     112.5)
```

FORTRAN IV program listing—Continued

```
  320 FORMAT (1H1,12HX VELOCITIES)
  330 FORMAT (1H ,25X,8HAT NODES/)
  340 FORMAT (1H0,25X,13HON BOUNDARIES/)
  350 FORMAT (1H ,10G12.3)
  360 FORMAT (1H1,12HY VELOCITIES)
  370 FORMAT (3H    ,11HTIM (N)   = ,1G12.5)
  380 FORMAT (3H    ,11HTIMEVELO = ,1G12.5)
  390 FORMAT (1H1,10X,29HSTABILITY CRITERIA --- M.O.C.//)
  400 FORMAT (1H0,8H VMAX = ,1PE9.2,5X,7HVMAY = ,1PE9.2)
  410 FORMAT (1H ,8H VMXBD= ,1PE9.2,5X,7HVMYBD= ,1PE9.2)
  420 FORMAT (1H0,8H TIMV = ,1PE9.2,5X,8HNTIMV = ,I5,5X,7HNMOV = ,I5/)
  430 FORMAT (1H0,8H TIMV = ,1PE9.2,5X,8HNTIMD = ,I5,5X,7HNMOV = ,I5)
  440 FORMAT (3H    ,11HTIMEDISP = ,1E12.5)
  450 FORMAT (1H1,32HDISPERSION EQUATION COEFFICIENTS,10X,25H=(D-IJ)*(B)
     1/(GRID FACTOR))
  460 FORMAT (1H ,35X,14HXX COEFFICIENT/)
  470 FORMAT (1H ,35X,14HYY COEFFICIENT/)
  480 FORMAT (1H ,35X,14HXY COEFFICIENT/)
  490 FORMAT (1H ,35X,14HYX COEFFICIENT/)
  500 FORMAT (1H ,1P10E8.1)
  510 FORMAT (2I4,2F10.1,2F10.7)
  520 FORMAT (8F10.7)
  530 FORMAT (1H0,10X,42HTHE LIMITING STABILITY CRITERION IS CELDIS)
  540 FORMAT (1HC,10X,40HTHE LIMITING STABILITY CRITERION IS BETA)
  550 FORMAT (1H0,10X,58HTHE LIMITING STABILITY CRITERION IS MAXIMUM INJ
     1ECTION RATE)
      END
      SUBROUTINE MOVE
      REAL *8TMRX,VPRM,HI,HR,HC,HK,WT,REC,RECH,TIM,AOPT,TITLE
      REAL *8XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /PRMI/ NTIM,NPMP,NPNT,NITP,N,NX,NY,NP,NREC,INT,NNX,NNY,NUMO
     1BS,NMOV,IMOV,NPMAX,ITMAX,NZCRIT,IPRNT,NPTPND,NPNTMV,NPNTVL,NPNTD,N
     2PNCHV,NPDELC
      COMMON /PRMK/ NODEID(20,20),NPCELL(20,20),LIMBO(500),IXOBS(5),IYOB
     1S(5)
      COMMON /HEDA/ THCK(20,20),PERM(20,20),TMWL(5,50),TMOBS(50),ANFCTR
      COMMON /HEDB/ TMRX(20,20,2),VPRM(20,20),HI(20,20),HR(20,20),HC(20,
     120),HK(20,20),WT(20,20),REC(20,20),RECH(20,20),TIM(100),AOPT(20),T
     2ITLE(10),XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /XINV/ DXINV,DYINV,ARINV,PORINV
      COMMON /CHMA/ PART(3,3200),CONC(20,20),TMCN(5,50),VX(20,20),VY(20,
     120),CONINT(20,20),CNRECH(20,20),POROS,SUMTCH,BETA,TIMV,STORM,STORM
     2I,CMSIN,CMSOUT,FLMIN,FLMOT,SUMIO,CELDIS,DLTRAT,CSTORM
      COMMON /CHMC/ SUMC(20,20),VXBDY(20,20),VYBDY(20,20)
      DIMENSION XNEW(4), YNEW(4), DIST(4)
C     ****************************************************************
      WRITE (6,680) NMOV
      SUMTCH=SUMT-TIM(N)
      F1=0.249
      IF (NPTPND.EQ.5) F1=0.299
      IF (NPTPND.EQ.9) F1=0.333
      CONST1=TIMV*DXINV
      CONST2=TIMV*DYINV
C     ---MOVE PARTICLES 'NMOV' TIMES---
      DO 650 IMOV=1,NMOV
   10 NPTM=NP
C         ---MOVE EACH PARTICLE---
      DO 590 IN=1,NP
      IF (PART(1,IN).EQ.0.0) GO TO 590
      KFLAG=0
C     ****************************************************************
C             ---COMPUTE OLD LOCATION---
```

FORTRAN IV program listing—Continued

```
      JFLAG=1
      IF (PART(1,IN).GT.0.0) GO TO 20
      JFLAG=-1
      PART(1,IN)=-PART(1,IN)
   20 XOLD=PART(1,IN)
      IX=XOLD+0.5
      IFLAG=1
      IF (PART(2,IN).GE.0.0) GO TO 30
      IFLAG=-1
      PART(2,IN)=-PART(2,IN)
   30 YOLD=PART(2,IN)
      IY=YOLD+0.5
      IF (THCK(IX,IY).EQ.0.0) GO TO 560
C     ****************************************************************
C           ---COMPUTE NEW LOCATION AND LOCATE CLOSEST NODE---
C           ---LOCATE NORTHWEST CORNER---
      IVX=XOLD
      IVY=YOLD
      IXE=IVX+1
      IYS=IVY+1
C     ****************************************************************
C        ---LOCATE QUADRANT, VEL. AT 4 CORNERS, CHECK FOR BOUNDARIES---
      CELDX=XOLD-IX
      CELDY=YOLD-IY
      IF (CELDX.EQ.0.0.AND.CELDY.EQ.0.0) GO TO 280
      IF (CELDX.GE.0.0.OR.CELDY.GE.0.0) GO TO 70
C              ---PT. IN NW QUADRANT---
      VXNW=VXBDY(IVX,IVY)
      VXNE=VX(IXE,IVY)
      VXSW=VXBDY(IVX,IYS)
      VXSE=VX(IXE,IYS)
      VYNW=VYBDY(IVX,IVY)
      VYNE=VYBDY(IXE,IVY)
      VYSW=VY(IVX,IYS)
      VYSE=VY(IXE,IYS)
      IF (THCK(IVX,IVY).EQ.0.0) GO TO 50
      IF (REC(IXE,IVY).EQ.0.0.AND.VPRM(IXE,IVY).LT.0.09) GO TO 40
      VXNE=VXNW
   40 IF (REC(IVX,IYS).EQ.0.0.AND.VPRM(IVX,IYS).LT.0.09) GO TO 50
      VYSW=VYNW
   50 IF (REC(IXE,IYS).EQ.0.0.AND.VPRM(IXE,IYS).LT.0.09) GO TO 270
      IF (THCK(IVX,IYS).EQ.0.0) GO TO 60
      VXSE=VXSW
   60 IF (THCK(IXE,IVY).EQ.0.0) GO TO 270
      VYSE=VYNE
      GO TO 270
C
   70 IF (CELDX.LE.0.0.OR.CELDY.GE.0.0) GO TO 130
C              ---PT. IN NE QUADRANT---
   80 VXNW=VX(IVX,IVY)
      VXNE=VXBDY(IVX,IVY)
      VXSW=VX(IVX,IYS)
      VXSE=VXBDY(IVX,IYS)
      VYNW=VYBDY(IVX,IVY)
      VYNE=VYBDY(IXE,IVY)
      VYSW=VY(IVX,IYS)
      VYSE=VY(IXE,IYS)
      IF (CELDX.EQ.0.0) GO TO 120
      IF (THCK(IXE,IVY).EQ.0.0) GO TO 100
      IF (REC(IVX,IVY).EQ.0.0.AND.VPRM(IVX,IVY).LT.0.09) GO TO 90
      VXNW=VXNE
   90 IF (REC(IXE,IYS).EQ.0.0.AND.VPRM(IXE,IYS).LT.0.09) GO TO 100
```

FORTRAN IV program listing—Continued

```
      VYSE=VYNE
  100 IF (REC(IVX,IYS).EQ.0.0.AND.VPRM(IVX,IYS).LT.0.09) GO TO 270
      IF (THCK(IXE,IYS).EQ.0.0) GO TO 110
      VXSW=VXSE
  110 IF (THCK(IVX,IVY).EQ.0.0) GO TO 270
      VYSW=VYNW
      GO TO 270
  120 IF (REC(IVX,IYS).EQ.0.0.AND.VPRM(IVX,IYS).LE.0.09) GO TO 270
      IF (THCK(IVX,IVY).EQ.0.0) GO TO 270
      VYSW=VYNW
      GO TO 270
C
  130 IF (CELDY.LE.0.0.OR.CELDX.GE.0.0) GO TO 190
C                ---PT. IN SW QUADRANT---
  140 VXNW=VXBDY(IVX,IVY)
      VXNE=VX(IXE,IVY)
      VXSW=VXBDY(IVX,IYS)
      VXSE=VX(IXE,IYS)
      VYNW=VY(IVX,IVY)
      VYNE=VY(IXE,IVY)
      VYSW=VYBDY(IVX,IVY)
      VYSE=VYBDY(IXE,IVY)
      IF (CELDY.EQ.0.0) GO TO 180
      IF (THCK(IVX,IYS).EQ.0.0) GO TO 160
      IF (REC(IVX,IVY).EQ.0.0.AND.VPRM(IVX,IVY).LT.0.09) GO TO 150
      VYNW=VYSW
  150 IF (REC(IXE,IYS).EQ.0.0.AND.VPRM(IXE,IYS).LT.0.09) GO TO 160
      VXSE=VXSW
  160 IF (REC(IXE,IVY).EQ.0.0.AND.VPRM(IXE,IVY).LT.0.09) GO TO 270
      IF (THCK(IVX,IVY).EQ.0.0) GO TO 170
      VXNE=VXNW
  170 IF (THCK(IXE,IYS).EQ.0.0) GO TO 270
      VYNE=VYSE
      GO TO 270
  180 IF (REC(IXE,IVY).EQ.0.0.AND.VPRM(IXE,IVY).LE.0.09) GO TO 270
      IF (THCK(IVX,IVY).EQ.0.0) GO TO 270
      VXNE=VXNW
      GO TO 270
C
  190 IF (CELDY.LE.0.0.OR.CELDX.LE.0.0) GO TO 260
C                ---PT. IN SE QUADRANT---
  200 VXNW=VX(IVX,IVY)
      VXNE=VXBDY(IVX,IVY)
      VXSW=VX(IVX,IYS)
      VXSE=VXBDY(IVX,IYS)
      VYNW=VY(IVX,IVY)
      VYNE=VY(IXE,IVY)
      VYSW=VYBDY(IVX,IVY)
      VYSE=VYBDY(IXE,IVY)
      IF (CELDY.EQ.0.0) GO TO 240
      IF (CELDX.EQ.0.0) GO TO 250
      IF (THCK(IXE,IYS).EQ.0.0) GO TO 220
      IF (REC(IXE,IVY).EQ.0.0.AND.VPRM(IXE,IVY).LT.0.09) GO TO 210
      VYNE=VYSE
  210 IF (REC(IVX,IYS).EQ.0.0.AND.VPRM(IVX,IYS).LT.0.09) GO TO 220
      VXSW=VXSE
  220 IF (REC(IVX,IVY).EQ.0.0.AND.VPRM(IVX,IVY).LT.0.09) GO TO 270
      IF (THCK(IXE,IVY).EQ.0.0) GO TO 230
      VXNW=VXNE
  230 IF (THCK(IVX,IYS).EQ.0.0) GO TO 270
      VYNW=VYSW
      GO TO 270
```

FORTRAN IV program listing—Continued

```
  240 IF (REC(IVX,IVY).EQ.0.0.AND.VPRM(IVX,IVY).LE.0.09) GO TO 270
      IF (THCK(IXE,IVY).EQ.0.0) GO TO 270
      VXNW=VXNE
      GO TO 270
  250 IF (REC(IVX,IVY).EQ.0.0.AND.VPRM(IVX,IVY).LE.0.09) GO TO 270
      IF (THCK(IVX,IYS).EQ.0.0) GO TO 270
      VYNW=VYSW
      GO TO 270
C
  260 IF (CELDX.EQ.0.0.AND.CELDY.LT.0.0) GO TO 80
      IF (CELDX.LT.0.0.AND.CELDY.EQ.0.0) GO TO 140
      IF (CELDX.GT.0.0.AND.CELDY.EQ.0.0) GO TO 200
      IF (CELDX.EQ.0.0.AND.CELDY.GT.0.0) GO TO 200
      WRITE (6,690) IN,IX,IY
  270 CONTINUE
C     *****************************************************************
C        ---BILINEAR INTERPOLATION---
      CELXD=XOLD-IVX
      CELDXH=AMOD(CELXD,0.5)
      CELDX=CELDXH*2.0
      CELDY=YOLD-IVY
C     *****************************************************************
C           ---X VELOCITY---
      VXN=VXNW*(1.0-CELDX)+VXNE*CELDX
      IF (THCK(IVX,IVY).EQ.0.0.OR.THCK(IXE,IVY).EQ.0.0) VXN=VXNW+VXNE
      VXS=VXSW*(1.0-CELDX)+VXSE*CELDX
      IF (THCK(IVX,IYS).EQ.0.0.OR.THCK(IXE,IYS).EQ.0.0) VXS=VXSW+VXSE
      XVEL=VXN*(1.0-CELDY)+VXS*CELDY
      IF (THCK(IVX,IVY).EQ.0.0.AND.THCK(IXE,IVY).EQ.0.0) XVEL=VXS
      IF (THCK(IVX,IYS).EQ.0.0.AND.THCK(IXE,IYS).EQ.0.0) XVEL=VXN
C           ---Y VELOCITY---
      CELDYH=AMOD(CELDY,0.5)
      CELDY=CELDYH*2.0
      VYW=VYNW*(1.0-CELDY)+VYSW*CELDY
      IF (THCK(IVX,IVY).EQ.0.0.OR.THCK(IVX,IYS).EQ.0.0) VYW=VYNW+VYSW
      VYE=VYNE*(1.0-CELDY)+VYSE*CELDY
      IF (THCK(IXE,IVY).EQ.0.0.OR.THCK(IXE,IYS).EQ.0.0) VYE=VYNE+VYSE
      YVEL=VYW*(1.0-CELXD)+VYE*CELXD
      IF (THCK(IVX,IVY).EQ.0.0.AND.THCK(IVX,IYS).EQ.0.0) YVEL=VYE
      IF (THCK(IXE,IVY).EQ.0.0.AND.THCK(IXE,IYS).EQ.0.0) YVEL=VYW
C
      GO TO 290
  280 XVEL=VX(IX,IY)
      YVEL=VY(IX,IY)
  290 DISTX=XVEL*CONST1
      DISTY=YVEL*CONST2
C     *****************************************************************
C        ---BOUNDARY CONDITIONS---
      TEMPX=XOLD+DISTX
      TEMPY=YOLD+DISTY
      INX=TEMPX+0.5
      INY=TEMPY+0.5
      IF (THCK(INX,INY).GT.0.0) GO TO 330
C     *****************************************************************
C           ---X BOUNDARY---
      IF (THCK(INX,IY).EQ.0.0) GO TO 300
      PART(1,IN)=TEMPX
      GO TO 310
  300 BEYON=TEMPX-IX
      IF (BEYON.LT.0.0) BEYON=BEYON+0.5
      IF (BEYON.GT.0.0) BEYON=BEYON-0.5
      PART(1,IN)=TEMPX-2.0*BEYON
```

FORTRAN IV program listing—Continued

```
      INX=PART(1,IN)+0.5
      TEMPX=PART(1,IN)
C     *****************************************************************
C           ---Y BOUNDARY---
  310 IF (THCK(INX,INY).EQ.0.0) GO TO 320
      PART(2,IN)=TEMPY
      GO TO 340
C     *****************************************************************
  320 BEYON=TEMPY-IY
      IF (BEYON.LT.0.0) BEYON=BEYON+0.5
      IF (BEYON.GT.0.0) BEYON=BEYON-0.5
      PART(2,IN)=TEMPY-2.0*BEYON
      INY=PART(2,IN)+0.5
      TEMPY=PART(2,IN)
      GO TO 340
  330 PART(1,IN)=TEMPX
      PART(2,IN)=TEMPY
  340 CONTINUE
C     ****************************************************************
C        ---SUM CONCENTRATIONS AND COUNT PARTICLES---
      SUMC(INX,INY)=SUMC(INX,INY)+PART(3,IN)
      NPCELL(INX,INY)=NPCELL(INX,INY)+1
C     *****************************************************************
C        ---CHECK FOR CHANGE IN CELL LOCATION---
      IF (IX.EQ.INX.AND.IY.EQ.INY) GO TO 580
C           ---CHECK FOR CONST.-HEAD BDY. OR SOURCE AT OLD LOCATION---
      IF (REC(IX,IY).LT.0.0) GO TO 350
      IF (REC(IX,IY).GT.0.0) GO TO 360
      IF (VPRM(IX,IY).LT.0.09) GO TO 540
      IF (WT(IX,IY).GT.HK(IX,IY)) GO TO 350
      IF (WT(IX,IY).LT.HK(IX,IY)) GO TO 360
      GO TO 540
C     *****************************************************************
C           ---CREATE NEW PARTICLES AT BOUNDARIES---
  350 IF (IFLAG.GT.0) GO TO 550
      KFLAG=1
  360 DO 370 IL=1,500
      IF (LIMBO(IL).EQ.0) GO TO 370
      IP=LIMBO(IL)
      IF (IP.LT.IN) GO TO 380
  370 CONTINUE
C     *****************************************************************
C           ---GENERATE NEW PARTICLE---
      IF (NPTM.EQ.NPMAX) GO TO 600
      NPTM=NPTM+1
      IP=NPTM
      GO TO 390
  380 LIMBO(IL)=0
C
  390 IF (KFLAG.EQ.0) GO TO 520
      IF (THCK(IX+1,IY).EQ.0.0.OR.THCK(IX-1,IY).EQ.0.0.OR.THCK(IX,IY+1).
     1EQ.0.0.OR.THCK(IX,IY-1).EQ.0.0) GO TO 520
      IF (THCK(IX+1,IY+1).EQ.0.0.OR.THCK(IX+1,IY-1).EQ.0.0.OR.THCK(IX-1,
     1IY+1).EQ.0.0.OR.THCK(IX-1,IY-1).EQ.0.0) GO TO 520
C             ---IF CENTER SOURCE---
      IF (JFLAG.LT.0) GO TO 500
      JJ=4
      AN=TEMPY-YOLD
      AD=TEMPX-XOLD
      DISTMV=SQRT((AD*AD)+(AN*AN))
      IF (AD.EQ.0.0) GO TO 410
      SLOPE=AN/AD
```

FORTRAN IV program listing—Continued

```
      BI=YOLD-SLOPE*XOLD
      XC1=IX-F1
      XC2=IX+F1
      YC1=IY-F1
      YC2=IY+F1
C             ---COMPUTE NEW COORDINATES AND VERIFY---
      DO 400 IK=1,4
      YNEW(IK)=0.0
      XNEW(IK)=0.0
  400 DIST(IK)=0.0
      YNEW(1)=(SLOPE*XC1)+BI
      XNEW(1)=XC1
      YNEW(2)=(SLOPE*XC2)+BI
      XNEW(2)=XC2
      IF (SLOPE.EQ.0.0) GO TO 420
      YNEW(3)=YC1
      XNEW(3)=(YC1-BI)/SLOPE
      YNEW(4)=YC2
      XNEW(4)=(YC2-BI)/SLOPE
      GO TO 430
  410 YNEW(1)=IY-F1
      XNEW(1)=XOLD
      YNEW(2)=IY+F1
      XNEW(2)=XOLD
  420 JJ=2
  430 DO 440 II=1,JJ
  440 DIST(II)=SQRT((XNEW(II)-TEMPX)**2+(YNEW(II)-TEMPY)**2)*1.00001
      IACC=0
      DISTCK=2.0
      DO 460 IG=1,JJ
      IF (DIST(IG).GE.DISTMV.AND.DIST(IG).LT.DISTCK) GO TO 450
      GO TO 460
  450 IXC=XNEW(IG)+0.50
      IYC=YNEW(IG)+0.50
      IF (IXC.NE.IX.OR.IYC.NE.IY) GO TO 460
      IACC=IG
      DISTCK=DIST(IG)
  460 CONTINUE
      IF (IACC.LT.1.OR.IACC.GT.4) GO TO 510
      IF (XNEW(IACC).EQ.XC1.OR.XNEW(IACC).EQ.XC2) GO TO 470
      IF (YNEW(IACC).EQ.YC1.OR.YNEW(IACC).EQ.YC2) GO TO 480
      GO TO 510
  470 IF (YNEW(IACC).LT.YC1) YNEW(IACC)=YC1
      IF (YNEW(IACC).GT.YC2) YNEW(IACC)=YC2
      GO TO 490
  480 IF (XNEW(IACC).LT.XC1) XNEW(IACC)=XC1
      IF (XNEW(IACC).GT.XC2) XNEW(IACC)=XC2
  490 PART(1,IP)=XNEW(IACC)
      PART(2,IP)=YNEW(IACC)
      GO TO 530
  500 PART(1,IP)=-IX
      PART(2,IP)=IY
      GO TO 530
  510 PART(1,IP)=XOLD
      PART(2,IP)=YOLD
      GO TO 530
C             ---IF EDGE SOURCE OR SINK---
C                ---X POSITION---
  520 DLX=INX-IX
      PART(1,IP)=TEMPX-DLX
C                ---Y POSITION---
      DLY=INY-IY
```

FORTRAN IV program listing—Continued

```
      PART(2,IP)=TEMPY-DLY
      IF (KFLAG.GT.0) GO TO 530
C             ---IF SINK---
      SUMC(IX,IY)=SUMC(IX,IY)+CONC(IX,IY)
      NPCELL(IX,IY)=NPCELL(IX,IY)+1
C
  530 PART(2,IP)=-PART(2,IP)
      PART(3,IP)=CONC(IX,IY)
      IF (REC(IX,IY).EQ.0.0) GO TO 540
C     ***************************************************************
C           ---CHECK FOR DISCHARGE BOUNDARY AT NEW LOCATION---
  540 IFLAG=1.0
  550 IF (VPRM(INX,INY).GT.0.09.AND.WT(INX,INY).LT.HK(INX,INY)) GO TO 56
     10
      IF (REC(INX,INY).GT.0.0) GO TO 560
      GO TO 590
C     ***************************************************************
C           ---PUT PT. IN LIMBO---
  560 PART(1,IN)=0.0
      PART(2,IN)=0.0
      PART(3,IN)=0.0
      DO 570 ID=1,500
      IF (LIMBO(ID).GT.0) GO TO 570
      LIMBO(ID)=IN
      GO TO 590
  570 CONTINUE
C
  580 IF (IFLAG.LT.0) PART(2,IN)=-TEMPY
      IF (JFLAG.LT.0) PART(1,IN)=-TEMPX
  590 CONTINUE
C     ---END OF LOOP---
C     ***************************************************************
      GO TO 620
C         ---RESTART MOVE IF PT. LIMIT EXCEEDED---
  600 WRITE (6,700) IMOV,IN
      TEST=100.0
      CALL GENPT
      DO 610 IX=1,NX
      DO 610 IY=1,NY
      SUMC(IX,IY)=0.0
  610 NPCELL(IX,IY)=0
      TEST=0.0
      GO TO 10
C     ***************************************************************
  620 SUMTCH=SUMTCH+TIMV
C         ---ADJUST NUMBER OF PARTICLES---
      NP=NPTM
      WRITE (6,670) NP,IMOV
C     ***************************************************************
      CALL CNCON
C     ***************************************************************
C         ---STORE OBS. WELL DATA FOR STEADY FLOW PROBLEMS---
      IF (S.GT.0.0) GO TO 640
      IF (NUMOBS.LE.0) GO TO 640
      J=MOD(IMOV,50)
      IF (J.EQ.0) J=50
      TMOBS(J)=SUMTCH
      DO 630 I=1,NUMOBS
      TMWL(I,J)=HK(IXOBS(I),IYOBS(I))
  630 TMCN(I,J)=CONC(IXOBS(I),IYOBS(I))
C         ---PRINT CHEMICAL OUTPUT---
  640 IF (IMOV.GE.NMOV) GO TO 660
```

FORTRAN IV program listing—Continued

```
  650 IF (MOD(IMOV,NPNTMV).EQ.0.OR.MOD(IMOV,50).EQ.0) CALL CHMOT
C     ******************************************************************
  660 RETURN
C     ******************************************************************
C
C
C
  670 FORMAT (1HC,2X,2HNP,7X,2H= ,8X,I4,10X,11HIMOV      = ,8X,I4)
  680 FORMAT (1H0,10X,61HNO. OF PARTICLE MOVES REQUIRED TO COMPLETE THIS
     1 TIME STEP  = ,I4//)
  690 FORMAT (1H0,5X,53H*** WARNING ***     QUADRANT NOT LOCATED FOR PT.
     1 NO. ,I5,11H , IN CELL ,2I4)
  700 FORMAT (1H0,5X,17H ***    NOTE    ***,10X,23HNPTM.EQ.NPMAX --- IMOV=
     1,I4,5X,8HPT. NO.=,I4,5X,10HCALL GENPT/)
      END
      SUBROUTINE CNCON
      REAL *8TMRX,VPRM,HI,HR,HC,HK,WT,REC,RECH,TIM,AOPT,TITLE
      REAL *8XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      REAL *8FLW
      COMMON /PRMI/ NTIM,NPMP,NPNT,NITP,N,NX,NY,NP,NREC,INT,NNX,NNY,NUMO
     1BS,NMOV,IMOV,NPMAX,ITMAX,NZCRIT,IPRNT,NPTPND,NPNTMV,NPNTVL,NPNTD,N
     2PNCHV,NPDELC
      COMMON /PRMK/ NODEID(20,20),NPCELL(20,20),LIMBO(500),IXOBS(5),IYOB
     1S(5)
      COMMON /HEDA/ THCK(20,20),PERM(20,20),TMWL(5,50),TMOBS(50),ANFCTR
      COMMON /HEDB/ TMRX(20,20,2),VPRM(20,20),HI(20,20),HR(20,20),HC(20,
     120),HK(20,20),WT(20,20),REC(20,20),RECH(20,20),TIM(100),AOPT(20),T
     2ITLE(10),XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /XINV/ DXINV,DYINV,ARINV,PORINV
      COMMON /CHMA/ PART(3,3200),CONC(20,20),TMCN(5,50),VX(20,20),VY(20,
     120),CONINT(20,20),CNRECH(20,20),POROS,SUMTCH,BETA,TIMV,STORM,STORM
     2I,CMSIN,CMSOUT,FLMIN,FLMOT,SUMIO,CELDIS,DLTRAT,CSTORM
      COMMON /DIFUS/ DISP(20,20,4)
      COMMON /CHMC/ SUMC(20,20),VXBDY(20,20),VYBDY(20,20)
      DIMENSION CNCNC(20,20), CNOLD(20,20)
C     ******************************************************************
      ITEST=0
      DO 10 IX=1,NX
      DO 10 IY=1,NY
      CNOLD(IX,IY)=CONC(IX,IY)
   10 CNCNC(IX,IY)=0.0
      APC=0.0
      NZERO=0
      TVA=AREA*TIMV
      ARPOR=AREA*POROS
C     ******************************************************************
C     ---CONC. CHANGE FOR 0.5*TIMV DUE TO:
C            RECHARGE, PUMPING, LEAKAGE, DIVERGENCE OF VELOCITY...
      CONST=0.5*TIMV
   20 DO 60 IX=1,NX
      DO 60 IY=1,NY
      IF (THCK(IX,IY).EQ.0.0) GO TO 60
      EQFCT1=CONST/THCK(IX,IY)
      EQFCT2=EQFCT1/POROS
      C1=CONC(IX,IY)
      CLKCN=0.0
      SLEAK=(HK(IX,IY)-WT(IX,IY))*VPRM(IX,IY)
      IF (SLEAK.LT.0.0) CLKCN=CNRECH(IX,IY)
      IF (SLEAK.GT.0.0) CLKCN=C1
      CNREC=C1
      RATE=REC(IX,IY)*ARINV
      IF (RATE.LT.0.0) CNREC=CNRECH(IX,IY)
```

FORTRAN IV program listing—Continued

```
      DIV=RATE+SLEAK+RECH(IX,IY)
      IF (S.EQ.0.0) GO TO 30
      DERH=(HK(IX,IY)-HR(IX,IY))/TIM(N)
      DIV=DIV+S*DERH
      IF (S.LT.0.005) GO TO 30
C     ...NOTE: ABOVE STATEMENT ASSUMES THAT S=0.005 SEPARATES CONFINED
C              FROM UNCONFINED CONDITIONS; THIS CRITERION SHOULD BE
C              CHANGED IF FIELD CONDITIONS ARE DIFFERENT.
      DELC=EQFCT2*(C1*(DIV-POROS*DERH)-RATE*CNREC-SLEAK*CLKCN-RECH(IX,IY
     1)*CNRECH(IX,IY))
      GO TO 40
   30 DELC=EQFCT2*(C1*DIV-RATE*CNREC-SLEAK*CLKCN-RECH(IX,IY)*CNRECH(IX,I
     1Y))
   40 CNCNC(IX,IY)=CNCNC(IX,IY)+DELC
C     ---CONC. CHANGE DUE TO DISPERSION FOR 0.5*TIMV---
C        ---DISPERSION WITH TENSOR COEFFICIENTS---
      IF (BETA.EQ.0.0) GO TO 50
      X1=DISP(IX,IY,1)*(CONC(IX+1,IY)-C1)
      X2=DISP(IX-1,IY,1)*(CONC(IX-1,IY)-C1)
      Y1=DISP(IX,IY,2)*(CONC(IX,IY+1)-C1)
      Y2=DISP(IX,IY-1,2)*(CONC(IX,IY-1)-C1)
      XX1=DISP(IX,IY,3)*(CONC(IX,IY+1)+CONC(IX+1,IY+1)-CONC(IX,IY-1)-CON
     1C(IX+1,IY-1))
      XX2=DISP(IX-1,IY,3)*(CONC(IX,IY+1)+CONC(IX-1,IY+1)-CONC(IX,IY-1)-C
     1ONC(IX-1,IY-1))
      YY1=DISP(IX,IY,4)*(CONC(IX+1,IY)+CONC(IX+1,IY+1)-CONC(IX-1,IY)-CON
     1C(IX-1,IY+1))
      YY2=DISP(IX,IY-1,4)*(CONC(IX+1,IY)+CONC(IX+1,IY-1)-CONC(IX-1,IY)-C
     1ONC(IX-1,IY-1))
   50 CNCNC(IX,IY)=CNCNC(IX,IY)+EQFCT1*(X1+X2+Y1+Y2+XX1-XX2+YY1-YY2)
   60 CONTINUE
C     ****************************************************************
      ITEST=ITEST+1
      IF (ITEST.EQ.1) GO TO 70
      GO TO 110
C     ****************************************************************
C     ---CONC. CHANGE AT NODES DUE TO CONVECTION---
   70 DO 90 IX=1,NX
      DO 90 IY=1,NY
      IF (THCK(IX,IY).EQ.0.0) GO TO 90
      APC=NPCELL(IX,IY)
      IF (APC.GT.0.0) GO TO 80
      IF (REC(IX,IY).NE.0.0.OR.VPRM(IX,IY).GT.0.09) GO TO 90
      NZERO=NZERO+1
      GO TO 90
   80 CONC(IX,IY)=SUMC(IX,IY)/APC
   90 CONTINUE
C        ---CHECK NUMBER OF CELLS VOID OF PTS.---
      IF (NZERO.GT.0) WRITE (6,290) NZERO,IMOV
      IF (NZERO.LE.NZCRIT) GO TO 20
      TEST=99.0
      WRITE (6,300)
      WRITE (6,320)
      DO 100 IY=1,NY
  100 WRITE (6,330) (NPCELL(IX,IY),IX=1,NX)
      GO TO 20
C     ****************************************************************
C     ---CHANGE CONCENTRATIONS AT NODES---
  110 DO 130 IX=1,NX
      DO 130 IY=1,NY
      IF (THCK(IX,IY).EQ.0.0) GO TO 120
      CONC(IX,IY)=CONC(IX,IY)+CNCNC(IX,IY)
```

FORTRAN IV program listing—Continued

```
      NPCELL(IX,IY)=0
      SUMC(IX,IY)=0.0
      IF (CONC(IX,IY).LE.0.0) GO TO 130
      CNCPCT=CNCNC(IX,IY)/CONC(IX,IY)
      SUMC(IX,IY)=CNCPCT
      GO TO 130
  120 IF (CONC(IX,IY).GT.0.0) WRITE (6,310) IX,IY,CONC(IX,IY)
      CONC(IX,IY)=0.0
  130 CONTINUE
C     ****************************************************************
C     ---CHANGE CONCENTRATION OF PARTICLES---
      DO 180 IN=1,NP
      IF (PART(1,IN).EQ.0.0) GO TO 180
      INX=ABS(PART(1,IN))+0.5
      INY=ABS(PART(2,IN))+0.5
C     ---UPDATE CONC. OF PTS. IN SINK/SOURCE CELLS---
      IF (REC(INX,INY).NE.0.0) GO TO 140
      IF (VPRM(INX,INY).LE.0.09) GO TO 150
  140 PART(3,IN)=CONC(INX,INY)
      GO TO 180
  150 IF (CNCNC(INX,INY).LT.0.0) GO TO 170
  160 PART(3,IN)=PART(3,IN)+CNCNC(INX,INY)
      GO TO 180
  170 IF (CONC(INX,INY).LE.0.0) GO TO 160
      IF (SUMC(INX,INY).LT.-1.0) GO TO 160
      PART(3,IN)=PART(3,IN)+PART(3,IN)*SUMC(INX,INY)
  180 CONTINUE
      WRITE (6,280) TIM(N),TIMV,SUMTCH
C     ****************************************************************
C     ---COMPUTE MASS BALANCE FOR SOLUTE---
      CSTORM=0.0
      STORM=0.0
      DO 270 IX=1,NX
      DO 270 IY=1,NY
      IF (THCK(IX,IY).EQ.0.0) GO TO 270
      SUMC(IX,IY)=0.0
C        ---COMPUTE MASS OF SOLUTE IN STORAGE---
      STORM=STORM+CONC(IX,IY)*THCK(IX,IY)*ARPOR
C        ---ACCOUNT FOR MASS PUMPED IN, OUT, RECHARGED, & DISCHARGED---
      IF (REC(IX,IY)) 200,210,190
  190 CMSOUT=CMSOUT+REC(IX,IY)*CNOLD(IX,IY)*TIMV
      GO TO 210
  200 CMSIN=CMSIN+REC(IX,IY)*CNRECH(IX,IY)*TIMV
  210 IF (RECH(IX,IY)) 230,240,220
  220 CMSOUT=CMSOUT+RECH(IX,IY)*CNOLD(IX,IY)*TVA
      GO TO 240
  230 CMSIN=CMSIN+RECH(IX,IY)*CNRECH(IX,IY)*TVA
C     ****************************************************************
C        ---ACCOUNT FOR BOUNDARY FLOW---
  240 IF (VPRM(IX,IY).EQ.0.0) GO TO 270
      FLW=VPRM(IX,IY)*(WT(IX,IY)-HK(IX,IY))
      IF (FLW.GT.0.0) GO TO 250
      IF (FLW.LT.0.0) GO TO 260
      GO TO 270
C           ---MASS IN BOUNDARY DURING TIME STEP---
  250 FLMIN=FLMIN+FLW*CNRECH(IX,IY)*TVA
      GO TO 270
C           ---MASS OUT DURING TIME STEP---
  260 FLMOT=FLMOT+FLW*CNOLD(IX,IY)*TVA
  270 CONTINUE
C     ****************************************************************
C        ---COMPUTE CHANGE IN MASS OF SOLUTE STORED---
```

FORTRAN IV program listing—Continued

```
      CSTORM=STORM-STORMI
      SUMIO=FLMIN+FLMOT-CMSIN-CMSOUT
C     *****************************************************************
C     ---REGENERATE PARTICLES IF 'NZCRIT' EXCEEDED---
      IF (TEST.GT.98.0) CALL GENPT
      TEST=0.0
C     *****************************************************************
      RETURN
C     *****************************************************************
C
C
C
  280 FORMAT (3H   ,11HTIM(N)    = ,1G12.5,10X,11HTIMV      = ,1G12.5,10X,
     19HSUMTCH = ,G12.5)
  290 FORMAT (1H0,5X,40HNUMBER OF CELLS WITH ZERO PARTICLES   =   ,I4,5X,9
     1HIMOV   =   ,I4/)
  300 FORMAT (1H0,5X,44H***    NZCRIT EXCEEDED   ---   CALL GENPT    ***/)
  310 FORMAT (1H ,5X,37H***CONC.GT.0.AND.THCK.EQ.0 AT NODE = ,2I4,4X,7HC
     1ONC = ,G10.4,4H ***)
  320 FORMAT (1H0,2X,6HNPCELL/)
  330 FORMAT (1H ,4X,20I3)
      END
      SUBROUTINE OUTPT
      REAL *8TMRX,VPRM,HI,HR,HC,HK,WT,REC,RECH,TIM,AOPT,TITLE
      REAL *8XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /PRMI/ NTIM,NPMP,NPNT,NITP,N,NX,NY,NP,NREC,INT,NNX,NNY,NUMO
     1BS,NMOV,IMOV,NPMAX,ITMAX,NZCRIT,IPRNT,NPTPND,NPNTMV,NPNTVL,NPNTD,N
     2PNCHV,NPDELC
      COMMON /PRMK/ NODEID(20,20),NPCELL(20,20),LIMBO(500),IXOBS(5),IYOB
     1S(5)
      COMMON /HEDA/ THCK(20,20),PERM(20,20),TMWL(5,50),TMOBS(50),ANFCTR
      COMMON /HEDB/ TMRX(20,20,2),VPRM(20,20),HI(20,20),HR(20,20),HC(20,
     120),HK(20,20),WT(20,20),REC(20,20),RECH(20,20),TIM(100),AOPT(20),T
     2ITLE(10),XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /BALM/ TOTLQ
      DIMENSION IH(20)
C     *****************************************************************
      TIMD=SUMT/86400.
      TIMY=SUMT/(86400.0*365.25)
C     ---PRINT HEAD VALUES---
      WRITE (6,120)
      WRITE (6,130) N
      WRITE (6,140) SUMT
      WRITE (6,150) TIMD
      WRITE (6,160) TIMY
      WRITE (6,170)
      DO 10 IY=1,NY
   10 WRITE (6,180) (HK(IX,IY),IX=1,NX)
      IF (N.EQ.0) GO TO 110
C     *****************************************************************
C     ---PRINT HEAD MAP---
      WRITE (6,120)
      WRITE (6,130) N
      WRITE (6,140) SUMT
      WRITE (6,150) TIMD
      WRITE (6,160) TIMY
      WRITE (6,170)
      DO 30 IY=1,NY
      DO 20 IX=1,NX
   20 IH(IX)=HK(IX,IY)+0.5
   30 WRITE (6,190) (IH(ID),ID=1,NX)
C     *****************************************************************
```

FORTRAN IV program listing—Continued

```
C      ---COMPUTE WATER BALANCE AND DRAWDOWN---
       QSTR=0.0
       PUMP=0.0
       TPUM=0.0
       QIN=0.0
       QOUT=0.0
       QNET=0.0
       DELQ=0.0
       JCK=0
       PCTERR=0.0
       WRITE (6,290)
C
       DO 80 IY=1,NY
       DO 70 IX=1,NX
       IH(IX)=0.0
       IF (THCK(IX,IY).EQ.0.0) GO TO 70
       TPUM=REC(IX,IY)+RECH(IX,IY)*AREA+TPUM
       IF (VPRM(IX,IY).EQ.0.0) GO TO 60
       DELQ=VPRM(IX,IY)*AREA*(WT(IX,IY)-HK(IX,IY))
       IF (DELQ.GT.0.0) GO TO 40
       QOUT=QOUT+DELQ
       GO TO 50
   40  QIN=QIN+DELQ
   50  QNET=QNET+DELQ
   60  DDRW=HI(IX,IY)-HK(IX,IY)
       IH(IX)=DDRW+0.5
       QSTR=QSTR+DDRW*AREA*S
   70  CONTINUE
C         ---PRINT DRAWDOWN MAP---
       WRITE (6,300) (IH(IX),IX=1,NX)
   80  CONTINUE
       PUMP=TPUM*SUMT
       DELS=-QSTR/SUMT
       ERRMB=PUMP-TOTLQ-QSTR
       DEN=PUMP+TOTLQ
       IF (ABS(DEN).EQ.ABS(ERRMB)) JCK=1
       IF (DEN.EQ.0.0) GO TO 100
       IF (JCK.EQ.1) GO TO 90
       PCTERR=ERRMB*200.0/DEN
       GO TO 100
   90  IF (QIN.EQ.0.0) GO TO 100
       PCTERR=100.0*QNET/QIN
C         ---PRINT MASS BALANCE DATA FOR FLOW MODEL---
  100  WRITE (6,240)
       WRITE (6,250) PUMP
       WRITE (6,230) QSTR
       WRITE (6,260) TOTLQ
       WRITE (6,270) ERRME
       IF (JCK.EQ.0) WRITE (6,280) PCTERR
       WRITE (6,200) QIN,QOUT,QNET
       WRITE (6,210) TPUM
       WRITE (6,220) DELS
       IF (JCK.EQ.1) WRITE (6,280) PCTERR
C      ****************************************************************
  110  RETURN
C      ****************************************************************
C
C
C
  120  FORMAT (1H1,23HHEAD DISTRIBUTION - ROW)
  130  FOKMAT (1X,23HNUMBEK OF TIME STEPS = ,I15)
  140  FORMAT (8X,16HTIME(SECONDS) = ,1G12.5)
```

FORTRAN IV program listing—Continued

```
  150 FORMAT (8X,16HTIME(DAYS)     = ,1E12.5)
  160 FORMAT (8X,16HTIME(YEARS)    = ,1E12.5)
  170 FORMAT (1H )
  180 FORMAT (1H0,10F12.7/10F12.7)
  190 FORMAT (1H0,20I4)
  200 FORMAT (1H0,2X,33HRATE MASS BALANCE -- (IN C.F.S.) //10X,8HQIN  =
     1 ,G12.5/10X,8HQOUT =  ,G12.5/10X,8HQNET =  ,G12.5/)
  210 FORMAT (1H ,17X,8HTPUM =  ,G12.5)
  220 FORMAT (1H ,17X,8HDELS =  ,G12.5/)
  230 FORMAT (4X,29HWATER RELEASE FROM STORAGE = ,1E12.5)
  240 FORMAT (1H0,2X,23HCUMULATIVE MASS BALANCE//)
  250 FORMAT (4X,29HCUMULATIVE  NET  PUMPAGE   = ,1E12.5)
  260 FORMAT (4X,29HCUMULATIVE  NET  LEAKAGE   = ,1E12.5)
  270 FORMAT (1H0,7X,25HMASS BALANCE RESIDUAL  = ,G12.5)
  280 FORMAT (1H ,7X,25HERROR  (AS PERCENT)    = ,G12.5/)
  290 FORMAT (1H1,8HDRAWDOWN)
  300 FORMAT (3H   ,20I5)
      END
      SUBROUTINE CHMOT
      REAL *8TMRX,VPRM,HI,HR,HC,HK,WT,REC,RECH,TIM,AOPT,TITLE
      REAL *8XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /PRMI/ NTIM,NPMP,NPNT,NITP,N,NX,NY,NP,NREC,INT,NNX,NNY,NUMO
     1BS,NMOV,IMOV,NPMAX,ITMAX,NZCRIT,IPRNT,NPTPND,NPNTMV,NPNTVL,NPNTD,N
     2PNCHV,NPDELC
      COMMON /PRMK/ NODEID(20,20),NPCELL(20,20),LIMBO(500),IXOBS(5),IYOB
     1S(5)
      COMMON /HEDA/ THCK(20,20),PERM(20,20),TMWL(5,50),TMOBS(50),ANFCTR
      COMMON /HEDB/ TMRX(20,20,2),VPRM(20,20),HI(20,20),HR(20,20),HC(20,
     120),HK(20,20),WT(20,20),REC(20,20),RECH(20,20),TIM(100),AOPT(20),T
     2ITLE(10),XDEL,YDEL,S,AREA,SUMT,RHO,PARAM,TEST,TOL,PINT,HMIN,PYR
      COMMON /CHMA/ PART(3,3200),CONC(20,20),TMCN(5,50),VX(20,20),VY(20,
     120),CONINT(20,20),CNRECH(20,20),POROS,SUMTCH,BETA,TIMV,STORM,STORM
     2I,CMSIN,CMSOUT,FLMIN,FLMOT,SUMIO,CELDIS,DLTRAT,CSTORM
      DIMENSION IC(20)
C     *****************************************************************
      TMFY=86400.0*365.25
      TMYR=SUMT/TMFY
      TCHD=SUMTCH/86400.0
      TCHYR=SUMTCH/TMFY
      IF (IPRNT.GT.0) GO TO 100
C     *****************************************************************
C     ---PRINT CONCENTRATIONS---
      WRITE (6,160)
      WRITE (6,170) N
      IF (N.GT.0) WRITE (6,180) TIM(N)
      WRITE (6,190) SUMT
      WRITE (6,450) SUMTCH
      WRITE (6,200) TCHD
      WRITE (6,210) TMYR
      WRITE (6,460) TCHYR
      WRITE (6,380) IMOV
      WRITE (6,220)
      DO 20 IY=1,NY
      DO 10 IX=1,NX
   10 IC(IX)=CONC(IX,IY)+0.5
   20 WRITE (6,240) (IC(IX),IX=1,NX)
C     *****************************************************************
      IF (N.EQ.0) GO TO 150
      IF (NPDELC.EQ.0) GO TO 50
C
C     ---PRINT CHANGES IN CONCENTRATION---
      WRITE (6,230)
```

FORTRAN IV program listing—Continued

```
      WRITE (6,170) N
      WRITE (6,180) TIM(N)
      WRITE (6,190) SUMT
      WRITE (6,450) SUMTCH
      WRITE (6,200) TCHD
      WRITE (6,210) TMYR
      WRITE (6,460) TCHYR
      WRITE (6,380) IMOV
      WRITE (6,220)
      DO 40 IY=1,NY
      DO 30 IX=1,NX
      CNG=CONC(IX,IY)-CONINT(IX,IY)
   30 IC(IX)=CNG
   40 WRITE (6,240) (IC(IX),IX=1,NX)
C     ****************************************************************
C     ---PRINT MASS BALANCE DATA FOR SOLUTE---
   50 RESID=SUMIO-CSTORM
      IF (SUMIO.EQ.0.0) GO TO 60
      RESID=SUMIO-CSTORM
      ERR1=RESID*200.0/(SUMIO+CSTORM)
   60 IF (STORMI.EQ.0.0) GO TO 70
      ERR3=-100.0*RESID/(STORMI-SUMIO)
   70 WRITE (6,220)
      WRITE (6,250)
      WRITE (6,220)
      WRITE (6,260) FLMIN
      WRITE (6,270) FLMOT
      RECIN=-CMSIN
      RECOUT=-CMSOUT
      WRITE (6,290) RECIN
      WRITE (6,280) RECOUT
      WRITE (6,300) SUMIO
      WRITE (6,310) STORMI
      WRITE (6,320) STORM
      WRITE (6,330) CSTORM
      IF (SUMIO.EQ.0.0) GO TO 80
      WRITE (6,340)
      WRITE (6,350) RESID
      WRITE (6,360) ERR1
   80 IF (STORMI.EQ.0.0) GO TO 90
      WRITE (6,370)
      WRITE (6,360) ERR3
C     ****************************************************************
C     ---PRINT HYDROGRAPHS AFTER 50 STEPS OR END OF SIMULATION---
   90 IF (MOD(IMOV,50).EQ.0.AND.S.EQ.0.0) GO TO 100
      IF (MOD(N,50).EQ.0.AND.S.GT.0.0) GO TO 100
      GO TO 150
  100 WRITE (6,390) TITLE
      IF (NUMOBS.LE.0) GO TO 150
      WRITE (6,400) INT
      IF (S.GT.0.0) WRITE (6,410)
      IF (S.EQ.0.0) WRITE (6,420)
C        ---TABULATE HYDROGRAPH DATA---
      MOZ=0
      IF (S.GT.0.0) GO TO 110
      NTO=NMOV
      IF (NMOV.GT.50) NTO=MOD(IMOV,50)
      GO TO 120
  110 NTO=NTIM
      IF (NTIM.GT.50) NTO=MOD(N,50)
  120 IF (NTO.EQ.0) NTO=50
      DO 140 J=1,NUMOBS
```

FORTRAN IV program listing—Continued

```
      TMYR=0.0
      WRITE (6,430) J,IXOBS(J),IYOBS(J)
      WRITE (6,440) MOZ,WT(IXOBS(J),IYOBS(J)),CONINT(IXOBS(J),IYOBS(J)),
     1TMYR
      DO 130 M=1,NTO
      TMYR=TMOBS(M)/TMFY
  130 WRITE (6,440) M,TMWL(J,M),TMCN(J,M),TMYR
  140 CONTINUE
C     ****************************************************************
  150 RETURN
C     ****************************************************************
C
C
C
  160 FORMAT (1H1,13HCONCENTRATION/)
  170 FORMAT (1X,23HNUMBER OF TIME STEPS = ,1I5)
  180 FORMAT (8X,16HDELTA T       = ,1G12.5)
  190 FORMAT (8X,16HTIME(SECONDS) = ,1G12.5)
  200 FORMAT (3X,21HCHEM.TIME(DAYS)     = ,1E12.5)
  210 FORMAT (8X,16HTIME(YEARS)   = ,1E12.5)
  220 FORMAT (1H )
  230 FORMAT (1H1,23HCHANGE IN CONCENTRATION/)
  240 FORMAT (1H0,20I5)
  250 FORMAT (1H ,21HCHEMICAL MASS BALANCE)
  260 FORMAT (8X,25HMASS IN BOUNDARIES      = ,1E12.5)
  270 FORMAT (8X,25HMASS OUT BOUNDARIES     = ,1E12.5)
  280 FORMAT (8X,25HMASS PUMPED OUT         = ,1E12.5)
  290 FORMAT (8X,25HMASS PUMPED IN          = ,1E12.5)
  300 FORMAT (8X,25HINFLOW MINUS OUTFLOW    = ,1E12.5)
  310 FORMAT (8X,25HINITIAL MASS STORED     = ,1E12.5)
  320 FORMAT (8X,25HPRESENT MASS STORED     = ,1E12.5)
  330 FORMAT (8X,25HCHANGE MASS STORED      = ,1E12.5)
  340 FORMAT (1H ,5X,53HCOMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULA
     1TION:)
  350 FORMAT (8X,25HMASS BALANCE RESIDUAL   = ,1E12.5)
  360 FORMAT (8X,25HERROR  (AS PERCENT)     = ,1E12.5)
  370 FORMAT (1H ,5X,55HCOMPARE INITIAL MASS STORED WITH CHANGE IN MASS
     1STORED:)
  380 FORMAT (1X,23H NO. MOVES COMPLETED = ,1I5)
  390 FORMAT (1H1,10A8//)
  400 FORMAT (1H0,5X,65HTIME VERSUS HEAD AND CONCENTRATION AT SELECTED O
     1BSERVATION POINTS//15X,19HPUMPING PERIOD NO. ,I4////)
  410 FORMAT (1H0,16X,19HTRANSIENT  SOLUTION////)
  420 FORMAT (1H0,15X,21HSTEADY-STATE SOLUTION////)
  430 FORMAT (1H0,20X,22HOBS.WELL NO.    X    Y,17X,1HN,6X,40HHEAD (FT)
     1   CONC.(MG/L)    TIME (YEARS)//24X,I3,9X,I2,3X,I2//)
  440 FORMAT (1H ,58X,I2,6X,F7.1,8X,F7.1,8X,F7.2)
  450 FORMAT (1H ,2X,21HCHEM.TIME(SECONDS) = ,E12.5)
  460 FORMAT (1H ,2X,21HCHEM.TIME(YEARS)   = ,E12.5)
      END
```

Attachment II

Definition of Selected Program Variables

AAQ	area of aquifer in model
ALNG	BETA
ANFCTR	anisotropy factor (ratio of T_{yy} to T_{xx})
AOPT	iteration parameters
AREA	area of one cell in finite-difference grid
BETA	longitudinal dispersivity of porous medium
CELDIS	maximum distance across one cell that a particle is permitted to move in one step (as fraction of width of cell)
CLKCN	concentration of leakage through confining layer or streambed
CMSIN	mass of solute recharged into aquifer
CMSOUT	mass of solute discharged from aquifer
CNCNC	change in concentration due to dispersion and sources
CNCPCT	change in concentration as percentage of concentration at node
CNOLD	concentration at node at end of previous time increment
CNREC	concentration of well withdrawal or injection
CNRECH	concentration in fluid source
CONC	concentration in aquifer at node
CONINT	concentration in aquifer at start of simulation
C1	CONC at node (IX,IY)
DALN	longitudinal dispersion coefficient
DDRW	drawdown
DELQ	volumetric rate of leakage across a confining layer or streambed
DELS	rate of change in ground-water storage
DERH	change in head with respect to time
DISP	dispersion equation coefficients
DISTX	distance particle moves in x-direction during time increment
DISTY	distance particle moves in y-direction during time increment
DLTRAT	ratio of transverse to longitudinal dispersivity
DTRN	transverse dispersion coefficient
FCTR	multiplication or conversion factor
FLMIN	solute mass entering modeled area during time step
FLMOT	solute mass leaving modeled area during time step
GRDX	hydraulic gradient in x-direction
GRDY	hydraulic gradient in y-direction
HC	head from column computation
HI	initial head in aquifer
HK	computed head at end of time step
HMIN	minimum iteration parameter
HR	head from row computation in subroutine ITERAT; elsewhere HR represents head from previous time step
IMOV	particle movement step number
INT	pumping period number
IPRNT	print control index for hydrographs
ITMAX	maximum permitted number of iterations
IXOBS	x-coordinate of observation point
IYOBS	y-coordinate of observation point
KOUNT	iteration number for ADIP
LIMBO	array for temporary storage of particles
N	time step number
NCA	number of aquifer nodes in model
NCODES	number of node identification codes
NITP	number of iteration parameters
NMOV	number of particle movements (or time increments) required to complete time step
NODEID	node identification code
NP	total number of active particles in grid
NPCELL	number of particles in a cell during time increment
NPMAX	maximum number of available particles
NPMP	number of pumping periods or simulation periods
NPNT	number of time steps between printouts
NPTPND	initial number of particles per node
NREC	number of pumping wells
NTIM	number of time steps
NUMOBS	number of observation wells
NX	number of nodes in x-direction
NY	number of nodes in y-direction
NZCRIT	maximum number of cells that can be void of particles
NZERO	number of cells that are void of particles at the end of a time increment
PARAM	iteration parameter for current iteration
PART	1. x-coordinate of particle; 2. y-coordinate of particle; 3. concentration of particle. Also note that the signs of coordinates are used as flags to store information on original location of particle.
PERM	hydraulic conductivity (in LT^{-1})
PINT	pumping period in years
POROS	effective porosity
PUMP	cumulative net pumpage
PYR	total duration of pumping period (in seconds)
QNET	net water flux (in L^3T^{-1})

Definition of selected program variables—Continued

QSTR	cumulative change in volume of water in storage
REC	point source or sink; negative for injection, positive for withdrawal (in L^3T^{-1})
RECH	diffuse recharge or discharge; negative for recharge, positive for discharge (in LT^{-1})
RN	range in concentration between regenerated particle and adjacent node having lower concentration
RP	range in concentration between regenerated particle and adjacent node having higher concentration
S	storage coefficient (or specific yield)
SLEAK	rate of leakage through confining layer or streambed
STORM	change in total solute mass in storage (by summation)
STORMI	initial mass of solute in storage
SUMC	summation of concentrations of all particles in a cell
SUMIO	change in total solute mass in storage (from inflows—outflows)
SUMT	total elapsed time (in seconds)
SUMTCH	cumulative elapsed time during particle moves (in seconds)
THCK	saturated thickness of aquifer
TIM	length of specific time step (in seconds)
TIMD	elapsed time in days
TIMY	elapsed time in years
TIMV	length of time increment for particle movement (in seconds)
TIMX	time step multiplier for transient flow problems
TINIT	size of initial time step for transient flow problems (in seconds)
TITLE	problem description
TMCN	computed concentrations at observation points
TMOBS	elapsed times for observation point records
TMRX	transmissivity coefficients (harmonic means on cell boundaries; forward values are stored)
TMWL	computed heads at observation points
TOL	convergence criteria (ADIP)
TOTLQ	cumulative net leakage through confining layer or streambed
TRAN	transverse dispersivity of porous medium
VMAX	maximum value of VX
VMAY	maximum value of VY
VMGE	magnitude of velocity vector
VMXBD	maximum value of VXBDY
VMYBD	maximum value of VYBDY
VPRM	initially used to read transmissivity values at nodes; then after line B2270, VPRM equals leakance factor for confining layer or streambed (vertical hydraulic conductivity/thickness). If VPRM≥0.09, then the program assumes that the node is a constant-head boundary and is flagged for subsequent special treatment in calculating convective transport.
VX	velocity in x-direction at a node
VXBDY	velocity in x-direction on a boundary between nodes
VY	velocity in y-direction at a node
VYBDY	velocity in y-direction on a boundary between nodes
WT	initial water-table or potentiometric elevation, or constant head in stream or source bed
XDEL	grid spacing in x-direction
XOLD	x-coordinate of particle at end of previous time increment
XVEL	velocity of particle in x-direction
YDEL	grid spacing in y-direction
YOLD	y-coordinate of particle at end of previous time increment
YVEL	velocity of particle in y-direction

Attachment III
Data Input Formats

Card	Column	Format	Variable	Definition
1	1–80	10A8	TITLE	Description of problem
2	1– 4	I4	NTIM	Maximum number of time steps in a pumping period (limit=100)*.
	5– 8	I4	NPMP	Number of pumping periods. Note that if NPMP>1, then data set 10 must be completed.
	9–12	I4	NX	Number of nodes in *x* direction (limit=20)*.
	13–16	I4	NY	Number of nodes in *y* direction (limit=20)*.
	17–20	I4	NPMAX	Maximum number of particles (limit=3200)*. (See eq 71.)
	21–24	I4	NPNT	Time-step interval for printing hydraulic and chemical output data.
	25–28	I4	NITP	Number of iteration parameters (usually 4≤NITP≤7).
	29–32	I4	NUMOBS	Number of observation points to be specified in a following data set (limit=5)*.
	33–36	I4	ITMAX	Maximum allowable number of iterations in ADIP (usually 100 ≤ITMAX≤200).
	37–40	I4	NREC	Number of pumping or injection wells to be specified in a following data set.
	41–44	I4	NPTPND	Initial number of particles per node (options=4, 5, 8, 9).
	45–48	I4	NCODES	Number of node identification codes to be specified in a following data set (limit=10)*.
	49–52	I4	NPNTMV	Particle movement interval (IMOV) for printing chemical output data. (Specify 0 to print only at end of time steps.)
	53–56	I4	NPNTVL	Option for printing computed velocities (0=do not print; 1=print for first time step; 2=print for all time steps).
	57–60	I4	NPNTD	Option for printing computed dispersion equation coefficients (option definition same as for NPNTVL).
	61–64	I4	NPDELC	Option for printing computed changes in concentration (0=do not print; 1=print).
	65–68	I4	NPNCHV	Option to punch velocity data (option definition same as for NPNTVL). When specified, program will punch on unit 7 the velocities at nodes.

See footnotes at end of table.

Data input formats—Continued

Card	Column	Format	Variable	Definition
3	1– 5	G5.0	PINT	Pumping period in years.
	6–10	G5.0	TOL	Convergence criteria in ADIP (usually TOL≤0.01).
	11–15	G5.0	POROS	Effective porosity.
	16–20	G5.0	BETA	Characteristic length, in feet (=longitudinal dispersivity).
	21–25	G5.0	S	Storage coefficient (set $S=0$ for steady flow problems).
	26–30	G5.0	TIMX	Time increment multiplier for transient flow problems. TIMX is disregarded if $S=0$.
	31–35	G5.0	TINIT	Size of initial time step in seconds. TINIT is disregarded if $S=0$.
	36–40	G5.0	XDEL	Width of finite-difference cell in x direction, in feet.
	41–45	G5.0	YDEL	Width in finite-difference cell in y direction, in feet.
	46–50	G5.0	DLTRAT	Ratio of transverse to longitudinal dispersivity.
	51–55	G5.0	CELDIS	Maximum cell distance per particle move (value between 0 and 1.0).
	56–60	G5.0	ANFCTR	Ratio of T_{yy} to T_{xx}.

Data set	Number of cards	Format	Variable	Definition
1	Value of NUMOBS (limit=5)*	2I2	IXOBS, IYOBS	x and y coordinates of observation points. This data set is eliminated if NUMOBS is specified as =0.
2	Value of NREC	2I2, 2G8.2	IX, IY, REC, CNRECH	x and y coordinates of pumping (+) or injection (−) wells, rate in ft³/s, and if an injection well, the concentration of injected water. This data set is eliminated if NREC=0.
3	a. 1	I1, G10.0	INPUT, FCTR	Parameter card † for transmissivity.
	b. Value of NY (limit=20)*	20G4.1	VPRM	Array for temporary storage of transmissivity data, in ft²/s. For an anisotropic aquifer, read in values of T_{xx} and the program will adjust for anisotropy by multiplying T_{yy} by ANFCTR.
4	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for THCK.
	b. Value of NY (limit=20)*	20G3.0	THCK	Saturated thickness of aquifer, in feet.
5	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for RECH.
	b. Value of NY (limit=20)*	20G4.1	RECH	Diffuse recharge (−) or discharge (+), in ft/s.
6	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for NODEID.
	b. Value of NY (limit=20)*	20I1	NODEID	Node identification matrix (used to define constant-head nodes or other boundary conditions and stresses).

See footnotes at end of table.

Data input formats—Continued

Data set	Number of cards	Format	Variable	Definition
7	Value of NCODES (limit=10)*	I2, 3G10.2, I2	ICODE, FCTR1, FCTR2, FCTR3, OVERRD	Instructions for using NODEID array. When NODEID=ICODE, program sets leakance=FCTR1, CNRECH=FCTR2, and if OVERRD is nonzero, RECH =FCTR3. Set OVERRD=0 to preserve values of RECH specified in data set 5.
8	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for WT.
	b. Value of NY (limit=20)*	20G4.0	WT	Initial water-table or potentiometric elevation, or constant head in stream or source bed, in feet.
9	a. 1	I1, G10.0	INPUT, FCTR	Parameter card† for CONC.
	b. Value of NY (limit=20)*	20G4.0	CONC	Initial concentration in aquifer.
10				This data set allows time step parameters, print options, and pumpage data to be revised for each pumping period of the simulation. Data set 10 is only used if NPMP >1. The sequence of cards in data set 10 must be repeated (NPMP −1) times (that is, data set 10 is required for each pumping period after the first).
	a. 1	I1	ICHK	Parameter to check whether any revisions are desired. Set ICHK=1 if data are to be revised, and then complete data set 10b and c. Set ICHK=0 if data are not to be revised for the next pumping period, and skip rest of data set 10.
	b. 1	10I4,3G5.0	NTIM, NPNT, NITP, ITMAX, NREC, NPNTMV, NPNTVL, NPNTD, NPDELC, NPNCHV, PINT, TIMX, TINIT	Thirteen parameters to be revised for next pumping period; the parameters were previously defined in the description of data cards 2 and 3. Only include this card if ICHK=1 in previous part a.
	c. Value of NREC	2I2, 2G8.2	IX, IY, REC, CNRECH	Revision of previously defined data set 2. Include part c only if ICHK=1 in previous part a and if NREC>0 in previous part b.

* These limits can be modified if necessary by changing the corresponding array dimensions in the COMMON statements of the program.

† The parameter card must be the first card of the indicated data sets. It is used to specify whether the parameter is constant and uniform, and can be defined by one value, or whether it varies in space and must be defined at each node. If INPUT=0, the data set has a constant value, which is defined by FCTR. If INPUT=1, the data set is read from cards as described by part b. Then FCTR is a multiplication factor for the values read in the data set.

Attachment IV
Input Data for Test Problem 3

```
Card 1      TEST PROBLEM NO. 3 (STEADY FLOW, 1 WELL, CONSTANT-HEAD BOUNDARIES)
Card 2         1    1    9   103200    1    7    2 100    1    9    2  10    1    0    0    0
Card 3        2.5.0001 0.30 100.  0.0  0.0  0.0 900. 900.  0.3 0.50  1.0
Data Set 1    5 4
              5 7
Data Set 2    4 7    1.0
Data Set 3  0   0.1
Data Set 4  0   20.0
Data Set 5  0   0.0
Data Set 6  1   1.0
            000000000
            022111220
            000000000
            000000000
            000000000
            000000000
            000000000
            000000000
            022222220
            000000000
Data Set 7    2    1.0         0.0         0.0       0
              1    1.0       100.0         0.0       0
Data Set 8  1   1.0
              0.0100.100.100.100.100.100.100. 0.0



              0.0 75.  75.  75.  75.  75.  75.  75. 0.0
Data Set 9  0   0.0
```

Attachment V
Selected Output for Test Problem 3

```
U.S.G.S. METHOD-OF-CHARACTERISTICS MODEL FOR SOLUTE TRANSPORT IN GROUND WATER

TEST PROBLEM NO. 3 (STEADY FLOW, 1 WELL, CONSTANT-HEAD BOUNDARIES)

                    I N P U T     D A T A

                      GRID DESCRIPTORS

             NX     (NUMBER OF COLUMNS)  =      9
             NY     (NUMBER OF ROWS)     =     10
             XDEL   (X-DISTANCE IN FEET) =   900.0
             YDEL   (Y-DISTANCE IN FEET) =   900.0

                      TIME  PARAMETERS

             NTIM   (MAX. NO. OF TIME STEPS)       =      1
             NPMP   (NO. OF PUMPING PERIODS)       =      1
             PINT   (PUMPING PERIOD IN YEARS)      =      2.50
             TIMX   (TIME INCREMENT MULTIPLIER)    =      0.00
             TINIT  (INITIAL TIME STEP IN SEC.)    =      0.

               HYDROLOGIC AND CHEMICAL PARAMETERS

             S        (STORAGE COEFFICIENT)        =       0.000000
             POROS    (EFFECTIVE POROSITY)         =       0.30
             BETA     (CHARACTERISTIC LENGTH)      =     100.0
             DLTRAT   (RATIO OF TRANSVERSE TO
                       LONGITUDINAL DISPERSIVITY)  =       0.30
             ANFCTR   (RATIO OF T-YY TO T-XX)      =       1.000000

                      EXECUTION PARAMETERS

             NITP   (NO. OF ITERATION PARAMETERS) =     7
             TOL    (CONVERGENCE CRITERIA - ADIP) =     0.0001
             ITMAX  (MAX.NO.OF ITERATIONS - ADIP) =   100
             CELDIS (MAX.CELL DISTANCE PER MOVE
                         OF PARTICLES - M.O.C.)   =     0.500
             NPMAX  (MAX. NO. OF PARTICLES)       =  3200
             NPTPND (NO. PARTICLES PER NODE)      =     9

                      PROGRAM OPTIONS

             NPNT   (TIME STEP INTERVAL FOR
                     COMPLETE PRINTOUT)         =     1
             NPNTMV (MOVE INTERVAL FOR CHEM.
                     CONCENTRATION PRINTOUT)    =    10
             NPNTVL (PRINT OPTION-VELOCITY
                     0=NO; 1=FIRST TIME STEP;
                     2=ALL TIME STEPS)          =     1
             NPNTD  (PRINT OPTION-DISP.COEF.
                     0=NO; 1=FIRST TIME STEP;
                     2=ALL TIME STEPS)          =     0
             NUMOBS (NO. OF OBSERVATION WELLS
                     FOR HYDROGRAPH PRINTOUT)   =     2
             NREC   (NO. OF PUMPING WELLS)      =     1
             NCODES (FOR NODE IDENT.)           =     2
             NPNCHV (PUNCH VELOCITIES)          =     0
             NPDELC (PRINT OPT.-CONC. CHANGE)   =     0
```

Selected output for test problem 3—Continued

STEADY-STATE FLOW

TIME INTERVAL (IN SEC) FOR SOLUTE-TRANSPORT SIMULATION = 0.78894d+08

LOCATION OF OBSERVATION WELLS

NO.	X	Y
1	5	4
2	5	7

LOCATION OF PUMPING WELLS

X	Y	RATE(IN CFS)	CONC.
4	7	1.00	0.0

AREA OF ONE CELL = 0.8100d+06

X-Y SPACING:
900.00
900.00

TRANSMISSIVITY MAP (FT*FT/SEC)

0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
0.00	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
0.00	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
0.00	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
0.00	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
0.00	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
0.00	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
0.00	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

AQUIFER THICKNESS (FT)

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0	0.0
0.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0	0.0
0.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0	0.0
0.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0	0.0
0.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0	0.0
0.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0	0.0
0.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0	0.0
0.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Selected output for test problem 3—Continued

```
DIFFUSE RECHARGE AND DISCHARGE (FT/SEC)
  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00
  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00
  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00
  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00
  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00
  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00
  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00
  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00
  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00
  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00  0.00d+00


PERMEABILTY MAP (FT/SEC)
  0.0000.0000.0000.0000.0000.0000.0000.0000.000
  0.0000.0050.0050.0050.0050.0050.0050.0050.000
  0.0000.0050.0050.0050.0050.0050.0050.0050.000
  0.0000.0050.0050.0050.0050.0050.0050.0050.000
  0.0000.0050.0050.0050.0050.0050.0050.0050.000
  0.0000.0050.0050.0050.0050.0050.0050.0050.000
  0.0000.0050.0050.0050.0050.0050.0050.0050.000
  0.0000.0050.0050.0050.0050.0050.0050.0050.000
  0.0000.0050.0050.0050.0050.0050.0050.0050.000
  0.0000.0000.0000.0000.0000.0000.0000.0000.000


          NO. OF FINITE-DIFFERENCE CELLS IN AQUIFER =   56

          AREA OF AQUIFER IN MODEL  =  0.45360e+08   SQ. FT.


          NZCRIT   (MAX. NO. OF CELLS THAT CAN BE VOID OF
                    PARTICLES; IF EXCEEDED, PARTICLES ARE REGENERATED)   =    1
```

Selected output for test problem 3—Continued

```
NODE IDENTIFICATION MAP


     0     0     0     0     0     0     0     0     0
     0     2     2     1     1     1     2     2     0
     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0
     0     2     2     2     2     2     2     2     0
     0     0     0     0     0     0     0     0     0

       NO. OF NODE IDENT. CODES SPECIFIED =  2

              THE FOLLOWING ASSIGNMENTS HAVE BEEN MADE:
     CODE NO.      LEAKANCE      SOURCE CONC.     RECHARGE

          2          0.100e+01          0.00

          1          0.100e+01        100.00



VERTICAL PERMEABILITY/THICKNESS (FT/(FT*SEC))
    0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
    0.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 0.00
    0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
    0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
    0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
    0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
    0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
    0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
    0.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 0.00
    0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00



WATER TABLE
     0.    0.    0.    0.    0.    0.    0.    0.    0.
     0.  100.  100.  100.  100.  100.  100.  100.    0.
     0.    0.    0.    0.    0.    0.    0.    0.    0.
     0.    0.    0.    0.    0.    0.    0.    0.    0.
     0.    0.    0.    0.    0.    0.    0.    0.    0.
     0.    0.    0.    0.    0.    0.    0.    0.    0.
     0.    0.    0.    0.    0.    0.    0.    0.    0.
     0.    0.    0.    0.    0.    0.    0.    0.    0.
     0.   75.   75.   75.   75.   75.   75.   75.    0.
     0.    0.    0.    0.    0.    0.    0.    0.    0.
```

Selected output for test problem 3—Continued

```
ITERATION PARAMETERS
          0.246740d-01
          0.457299d-01
          0.847539d-01
           .157080
           .291125
           .539560
           1.00000
          0.000000
          0.000000
          0.000000
          0.000000
          0.000000
          0.000000
          0.000000
          0.000000
          0.000000
          0.000000
          0.000000
          0.000000
          0.000000


CONCENTRATION

NUMBER OF TIME STEPS =       0
       TIME(SECONDS) =   0.00000
  CHEM.TIME(SECONDS) =   0.00000e+00
  CHEM.TIME(DAYS)    =   0.00000e+00
       TIME(YEARS)   =   0.00000e+00
  CHEM.TIME(YEARS)   =   0.00000e+00
 NO. MOVES COMPLETED =       0

    0    0    0    0    0    0    0    0    0

    0    0    0    0    0    0    0    0    0

    0    0    0    0    0    0    0    0    0

    0    0    0    0    0    0    0    0    0

    0    0    0    0    0    0    0    0    0

    0    0    0    0    0    0    0    0    0

    0    0    0    0    0    0    0    0    0

    0    0    0    0    0    0    0    0    0

    0    0    0    0    0    0    0    0    0

    0    0    0    0    0    0    0    0    0


 N =     1
 NUMBER OF ITERATIONS =    20
```

Selected output for test problem 3—Continued

```
HEAD DISTRIBUTION - ROW
NUMBER OF TIME STEPS =       1
      TIME(SECONDS) =   0.78894d+08
      TIME(DAYS)    =   0.91313e+03
      TIME(YEARS)   =   0.25000e+01

  0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000

  0.0000000  99.9999995  99.9999995  99.9999995  99.9999995  99.9999995  99.9999995  99.9999995   0.0000000

  0.0000000  95.9387858  95.9346978  95.9468712  95.9958792  96.0611455  96.1171357  96.1482887   0.0000000

  0.0000000  91.8816815  91.8531641  91.8569301  91.9755221  92.1315893  92.2591385  92.3277521   0.0000000

  0.0000000  87.8530674  87.7393101  87.6521342  87.9176617  88.2305223  88.4600398  88.5758019   0.0000000

  0.0000000  83.9382225  83.5988909  83.0946482  83.8124811  84.4128118  84.7747129  84.9396259   0.0000000

  0.0000000  80.3627221  79.6233998  77.3151005  79.8248158  80.8335448  81.2863911  81.4683757   0.0000000

  0.0000000  77.5265176  77.2168501  76.7175099  77.3381095  77.8101323  78.0688950  78.1790838   0.0000000

  0.0000000  75.0000003  75.0000003  75.0000002  75.0000003  75.0000003  75.0000004  75.0000004   0.0000000

  0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0000000

HEAD DISTRIBUTION - ROW
NUMBER OF TIME STEPS =       1
      TIME(SECONDS) =   0.78894d+08
      TIME(DAYS)    =   0.91313e+03
      TIME(YEARS)   =   0.25000e+01

  0   0   0   0   0   0   0   0   0

  0 100 100 100 100 100 100 100   0

  0  96  96  96  96  96  96  96   0

  0  92  92  92  92  92  92  92   0

  0  88  88  88  88  88  88  89   0

  0  84  84  83  84  84  85  85   0

  0  80  80  77  80  81  81  81   0

  0  78  77  77  77  78  78  78   0

  0  75  75  75  75  75  75  75   0

  0   0   0   0   0   0   0   0   0
```

Selected output for test problem 3—Continued

```
DRAWDOWN
     0    0    0    0    0    0    0    0    0
     0    0    0    0    0    0    0    0    0
     0  -95  -95  -95  -95  -95  -95  -95    0
     0  -91  -91  -91  -91  -91  -91  -91    0
     0  -87  -87  -87  -87  -87  -87  -88    0
     0  -83  -83  -82  -83  -83  -84  -84    0
     0  -79  -79  -76  -79  -80  -80  -80    0
     0  -77  -76  -76  -76  -77  -77  -77    0
     0    0    0    0    0    0    0    0    0
     0    0    0    0    0    0    0    0    0

  CUMULATIVE MASS BALANCE

   CUMULATIVE  NET  PUMPAGE    =  0.78894e+08
   WATER RELEASE FROM STORAGE  =  0.00000e+00
   CUMULATIVE  NET  LEAKAGE    =  0.78895e+08

      MASS BALANCE RESIDUAL   =  -767.00
      ERROR  (AS PERCENT)     = -0.97219e-03

  RATE MASS BALANCE -- (IN C.F.S.)
        QIN  =     2.7857
        QOUT =    -1.7857
        QNET =     1.0000

               TPUM =     1.0000
               DELS =    0.00000

X VELOCITIES
                         AT NODES

  0.000      0.000      0.000      0.000      0.000      0.000      0.000      0.000      0.000
  0.000      0.935e-14 -0.924e-14 -0.699e-13 -0.131e-12 -0.139e-12 -0.996e-13 -0.712e-13  0.000
  0.000      0.757e-07 -0.749e-07 -0.566e-06 -0.106e-05 -0.112e-05 -0.807e-06 -0.577e-06  0.000
  0.000      0.528e-06  0.229e-06 -0.113e-05 -0.254e-05 -0.263e-05 -0.182e-05 -0.127e-05  0.000
  0.000      0.211e-05  0.186e-05 -0.165e-05 -0.536e-05 -0.502e-05 -0.320e-05 -0.214e-05  0.000
  0.000      0.628e-05  0.781e-05 -0.198e-05 -0.122e-04 -0.891e-05 -0.488e-05 -0.305e-05  0.000
  0.000      0.137e-04  0.282e-04 -0.186e-05 -0.326e-04 -0.135e-04 -0.588e-05 -0.337e-05  0.000
  0.000      0.573e-05  0.749e-05 -0.112e-05 -0.101e-04 -0.677e-05 -0.342e-05 -0.204e-05  0.000
  0.000      0.708e-12  0.925e-12 -0.139e-12 -0.125e-11 -0.835e-12 -0.422e-12 -0.252e-12  0.000
  0.000      0.000      0.000      0.000      0.000      0.000      0.000      0.000      0.000

                         ON BOUNDARIES

  0.000      0.000      0.000      0.000      0.000      0.000      0.000      0.000      0.000
  0.000      0.935e-14 -0.278e-13 -0.112e-12 -0.149e-12 -0.128e-12 -0.712e-13  0.000      0.000
  0.000      0.757e-07 -0.225e-06 -0.908e-06 -0.121e-05 -0.104e-05 -0.577e-06  0.000      0.000
  0.000      0.528e-06 -0.697e-07 -0.220e-05 -0.289e-05 -0.236e-05 -0.127e-05  0.000      0.000
  0.000      0.211e-05  0.161e-05 -0.492e-05 -0.579e-05 -0.425e-05 -0.214e-05  0.000      0.000
  0.000      0.628e-05  0.934e-05 -0.133e-04 -0.111e-04 -0.670e-05 -0.305e-05  0.000      0.000
  0.000      0.137e-04  0.427e-04 -0.465e-04 -0.187e-04 -0.839e-05 -0.337e-05  0.000      0.000
  0.000      0.573e-05  0.925e-05 -0.115e-04 -0.874e-05 -0.479e-05 -0.204e-05  0.000      0.000
  0.000      0.708e-12  0.114e-11 -0.142e-11 -0.108e-11 -0.592e-12 -0.252e-12  0.000      0.000
  0.000      0.000      0.000      0.000      0.000      0.000      0.000      0.000      0.000
```

Selected output for test problem 3—Continued

Y VELOCITIES

AT NODES

0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.000	0.752e-04	0.753e-04	0.751e-04	0.742e-04	0.729e-04	0.719e-04	0.713e-04	0.000
0.000	0.752e-04	0.754e-04	0.754e-04	0.743e-04	0.729e-04	0.717e-04	0.710e-04	0.000
0.000	0.749e-04	0.759e-04	0.768e-04	0.748e-04	0.725e-04	0.709e-04	0.701e-04	0.000
0.000	0.736e-04	0.764e-04	0.811e-04	0.756e-04	0.715e-04	0.693e-04	0.684e-04	0.000
0.000	0.694e-04	0.751e-04	0.957e-04	0.749e-04	0.685e-04	0.664e-04	0.658e-04	0.000
0.000	0.594e-04	0.591e-04	0.590e-04	0.599e-04	0.611e-04	0.621e-04	0.626e-04	0.000
0.000	0.497e-04	0.428e-04	0.214e-04	0.447e-04	0.540e-04	0.582e-04	0.599e-04	0.000
0.000	0.468e-04	0.411e-04	0.318e-04	0.433e-04	0.520e-04	0.568e-04	0.589e-04	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

ON BOUNDARIES

0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.000	0.752e-04	0.753e-04	0.751e-04	0.742e-04	0.729e-04	0.719e-04	0.713e-04	0.000
0.000	0.751e-04	0.756e-04	0.757e-04	0.745e-04	0.728e-04	0.714e-04	0.708e-04	0.000
0.000	0.746e-04	0.762e-04	0.779e-04	0.751e-04	0.722e-04	0.704e-04	0.695e-04	0.000
0.000	0.725e-04	0.767e-04	0.844e-04	0.760e-04	0.707e-04	0.682e-04	0.673e-04	0.000
0.000	0.662e-04	0.736e-04	0.107e-03	0.738e-04	0.663e-04	0.646e-04	0.643e-04	0.000
0.000	0.525e-04	0.446e-04	0.111e-04	0.461e-04	0.560e-04	0.596e-04	0.609e-04	0.000
0.000	0.468e-04	0.411e-04	0.318e-04	0.433e-04	0.520e-04	0.568e-04	0.589e-04	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

```
        STABILITY CRITERIA --- M.O.C.


VMAX =   3.26e-05      VMAY =   9.57e-05
VMXBD=   4.65e-05      VMYBD=   1.07e-04
TMV (MAX. INJ.) =   0.11955e+08
TIMV (CELDIS)   =   0.42045e+07

TIMV =   4.20e+06      NTIMV =     18      NMOV =     19

 TIM (N)  =   0.78894d+08
 TIMEVELO =   0.41523e+07
 TIMEDISP =   0.30143e+08

TIMV =   4.15e+06      NTIMD =      2      NMOV =     19

        THE LIMITING STABILITY CRITERION IS CELDIS

        NO. OF PARTICLE MOVES REQUIRED TO COMPLETE THIS TIME STEP  =   19
```

Selected output for test problem 3—Continued

```
CONCENTRATION

NUMBER OF TIME STEPS =      1
       DELTA T        =  0.78894d+08
       TIME(SECONDS)  =  0.78894d+08
  CHEM.TIME(SECONDS)  =  0.78894e+08
  CHEM.TIME(DAYS)     =  0.91313e+03
       TIME(YEARS)    =  0.25000e+01
  CHEM.TIME(YEARS)    =  0.25000e+01
 NO. MOVES COMPLETED =     19

    0    0    0    0    0    0    0    0    0
    0    0    2   98  100   98    2    0    0
    0    0    4   96  100   96    4    0    0
    0    0    7   92   99   93    7    0    0
    0    0    9   89   96   88    9    0    0
    0    1   10   81   89   80   10    1    0
    0    1    8   56   73   46    8    1    0
    0    0    2   20   35   19    3    0    0
    0    0    0    1    5    3    0    0    0
    0    0    0    0    0    0    0    0    0

CHEMICAL MASS BALANCE

       MASS IN BOUNDARIES      =  0.94642e+10
       MASS OUT BOUNDARIES     = -0.13340e+08
       MASS PUMPED IN          =  0.00000e+00
       MASS PUMPED OUT         = -0.96281e+09
       INFLOW MINUS OUTFLOW    =  0.84881e+10
       INITIAL MASS STORED     =  0.00000e+00
       PRESENT MASS STORED     =  0.84631e+10
       CHANGE MASS STORED      =  0.84631e+10
     COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION:
       MASS BALANCE RESIDUAL   =  0.24910e+08
       ERROR  (AS PERCENT)     =  0.29390e+00
```

Selected output for test problem 3—Continued

TEST PROBLEM NO. 3 (STEADY FLOW, 1 WELL, CONSTANT-HEAD BOUNDARIES)

TIME VERSUS HEAD AND CONCENTRATION AT SELECTED OBSERVATION POINTS*

PUMPING PERIOD NO. 1

STEADY-STATE SOLUTION

OBS.WELL NO.	X	Y	N	HEAD (FT)	CONC.(MG/L)	TIME (YEARS)
1	5	4				
			0	0.0	0.0	0.00
			1	92.0	0.0	0.13
			2	92.0	0.2	0.26
			3	92.0	1.2	0.39
			4	92.0	2.9	0.53
			5	92.0	15.5	0.66
			6	92.0	33.0	0.79
			7	92.0	53.1	0.92
			8	92.0	64.6	1.05
			9	92.0	72.9	1.18
			10	92.0	79.8	1.32
			11	92.0	85.4	1.45
			12	92.0	89.4	1.58
			13	92.0	92.2	1.71
			14	92.0	94.3	1.84
			15	92.0	95.8	1.97
			16	92.0	97.0	2.11
			17	92.0	97.8	2.24
			18	92.0	98.4	2.37
			19	92.0	98.7	2.50

Selected output for test problem 3—Continued

OBS.WELL NO.	X	Y
. 2	5	7

N	HEAD (FT)	CONC.(MG/L)	TIME (YEARS)
0	0.0	0.0	0.00
1	79.8	0.0	0.13
2	79.8	0.0	0.26
3	79.8	0.0	0.39
4	79.8	0.0	0.53
5	79.8	0.0	0.66
6	79.8	0.0	0.79
7	79.8	0.1	0.92
8	79.8	0.2	1.05
9	79.8	0.6	1.18
10	79.8	1.7	1.32
11	79.8	4.8	1.45
12	79.8	8.2	1.58
13	79.8	14.3	1.71
14	79.8	27.0	1.84
15	79.8	38.2	1.97
16	79.8	49.4	2.11
17	79.8	51.1	2.24
18	79.8	67.2	2.37
19	79.8	73.0	2.50

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