CHAPTER 2
DERIVATION OF THE FINITE-DIFFERENCE EQUATION

Mathematical Model

The three-dimensional movement of ground water of constant density through porous earth material may be described by the partial-differential equation

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t}, \qquad (2\text{–}1)$$

where

K_{xx}, K_{yy}, and K_{zz} are values of hydraulic conductivity along the x, y, and z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity (L/T);

h is the potentiometric head (L);

W is a volumetric flux per unit volume representing sources and/or sinks of water, with $W<0.0$ for flow out of the ground-water system, and $W>0.0$ for flow into the system (T^{-1});

S_S is the specific storage of the porous material (L^{-1}); and

t is time (T).

For a derivation of equation 2–1 see for example Rushton and Redshaw (1979). In general, S_s, K_{xx}, K_{yy}, and K_{zz} may be functions of space ($S_s = S_s(x,y,z)$, $K_{xx} = K_{xx}(x,y,z)$, and so forth) and W may be a function of space and time ($W = W(x,y,z,t)$). Equation 2–1 describes ground-water flow under nonequilibrium conditions in a heterogeneous and anisotropic medium, provided the principal axes of hydraulic conductivity are aligned with the coordinate directions. Equation 2–1, together with specification of flow and/or head conditions at the boundaries of an aquifer system and specification of initial-head conditions, constitutes a mathematical representation of a ground-water flow system. A solution of equation 2–1, in an analytical sense, is an algebraic expression giving $h(x,y,z,t)$ such that, when the derivatives of h with respect to space and time are substituted into equation 2–1, the equation and its initial and boundary conditions are satisfied. A time-varying head distribution of this nature characterizes the flow system, in that it measures both the energy of flow and the volume of water in storage, and can be used to calculate directions and rates of movement.

Except for very simple systems, analytical solutions of equation 2–1 are rarely possible, so various numerical methods must be employed to obtain approximate solutions. One such approach is the finite-difference method, wherein the continuous system described by equation 2–1 is replaced by a finite set of discrete points in space and time, and the partial derivatives are replaced by terms calculated from the differences in head values at these points. The process leads to systems of simultaneous linear algebraic difference equations; their solution yields values of head at specific points and times. These values constitute an approximation to the time-varying head distribution that would be given by an analytical solution of the partial-differential equation of flow.

The finite-difference analog of equation 2–1 may be derived by applying the rules of difference calculus; however, in the discussion presented here, an alternative approach is used with the aim of simplifying the mathematical treatment and explaining the computational procedure in terms of familiar physical concepts regarding the flow system.

Discretization Convention

Figure 2–1 shows a spatial discretization of an aquifer system with a grid of blocks called cells, the locations of which are described in terms of rows, columns, and layers. An i,j,k indexing system is used. For a system consisting of "NROW" rows, "NCOL" columns, and "NLAY" layers, i is the row index, i = 1,2,. . . NROW; j is the column index, j = 1,2,. . . NCOL; and k is the layer index, k = 1,2,. . . NLAY. For example, figure 2–1 shows a system with NROW = 5, NCOL = 9, and NLAY = 5. In formulating the equations of the model, an assumption was made that layers would generally correspond to horizontal geohydrologic units or intervals. Thus in terms of Cartesian coordinates, the k index denotes changes along the vertical, z; because the convention followed in this model is to number layers from the top down, an increment in the k index corresponds to a decrease in elevation. Similarly, rows would be considered parallel to the x axis, so that increments in the row index, i, would correspond to decreases in y; and columns would be considered parallel to the y axis, so that increments in the column index, j, would correspond to increases in x. These conventions were followed in constructing figure 2–1; however, applications of the model requires only that rows and columns fall along consistent orthogonal directions within the layers, and does not require the designation of x, y, or z coordinate axes.

Within each cell there is a point called a "node" at which head is to be calculated. Many schemes for locating nodes in cells could be used; however, the finite-difference equation developed in the following section uses the block-centered formulation in which the nodes are at the center of the cells.

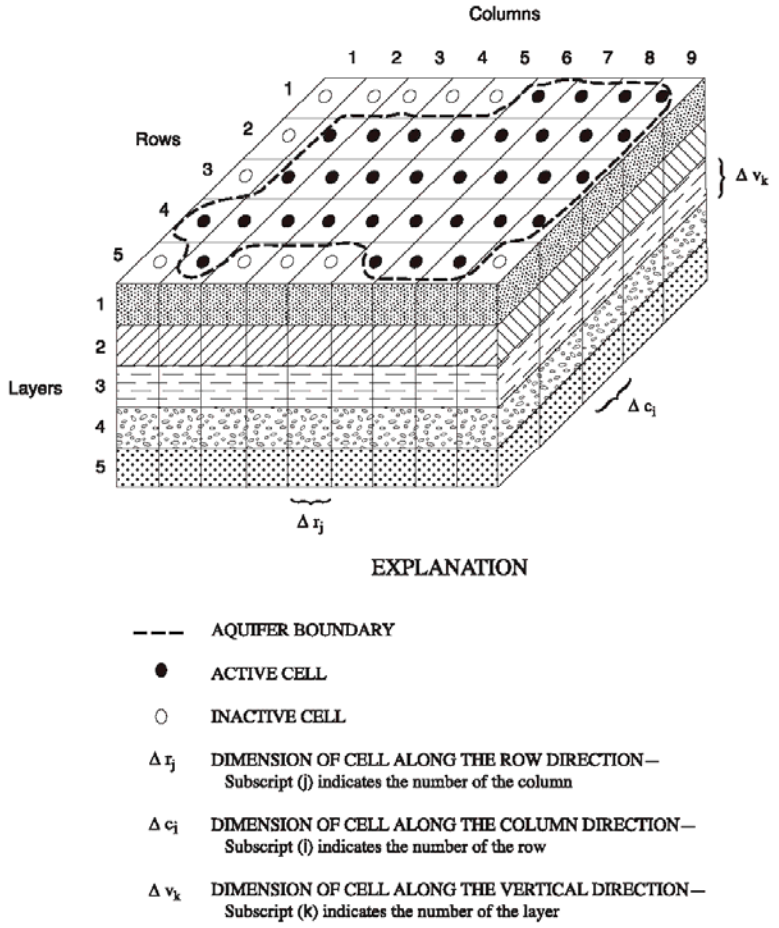

Figure 2–1. A discretized hypothetical aquifer system. (Modified from McDonald and Harbaugh, 1988.)

Following the conventions used in figure 2–1, the width of cells in the row direction, at a given column, j, is designated Δr_j; the width of cells in the column direction at a given row, i, is designated Δc_i; and the thickness of cells in a given layer, k, is designated Δv_k. Thus a cell with coordinates (i,j,k) = (4,8,3) has a volume of $\Delta r_8 \Delta c_4 \Delta v_3$. Note that in Cartesian coordinates with rows parallel to the x axis and columns parallel to the y axis, Δr_j would correspond to Δx_j, and Δc_i would correspond to Δy_i.

In the development of the finite-difference equation in the following section, the grid in MODFLOW is assumed to be rectangular horizontally and vertically. Later in this chapter (see Conceptual Aspects of Vertical Discretization) and in Chapter 5 (Internal Flow Packages), the possibility of vertical distortion of the grid is discussed.

In equation 2–1, the head, h, is a function of time as well as space so that, in the finite-difference formulation, discretization of the continuous time domain is also required. Time is broken into time steps, and head is calculated at each time step.

Finite-Difference Equation

Development of the ground-water flow equation in finite-difference form follows from the application of the continuity equation: the sum of all flows into and out of the cell must be equal to the rate of change in storage within the cell. Under the assumption that the density of ground water is constant, the continuity equation expressing the balance of flow for a cell is

$$\sum Q_i = SS \frac{\Delta h}{\Delta t} \Delta V \quad , \tag{2–2}$$

where

Q_i is a flow rate into the cell (L^3T^{-1});

SS has been introduced as the notation for specific storage in the finite-difference formulation; its definition is equivalent to that of S_s in equation 2–1—that is, SS is the volume of water that can be injected per unit volume of aquifer material per unit change in head (L^{-1});

ΔV is the volume of the cell (L^3); and

Δh is the change in head over a time interval of length Δt.

The term on the right-hand side is equivalent to the volume of water taken into storage over a time interval Δt given a change in head of Δh. Equation 2–2 is stated in terms of inflow and storage gain. Outflow and loss are represented by defining outflow as negative inflow and loss as negative gain.

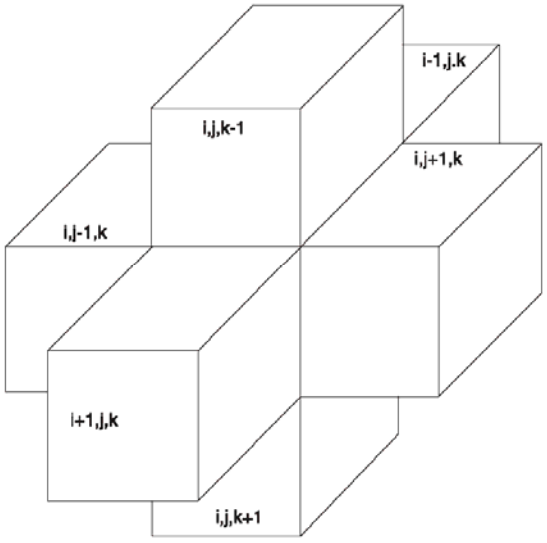

Figure 2–2. Indicies for the six adjacent cells surrounding cell i,j,k (hidden). (Modified from McDonald and Harbaugh, 1988.)

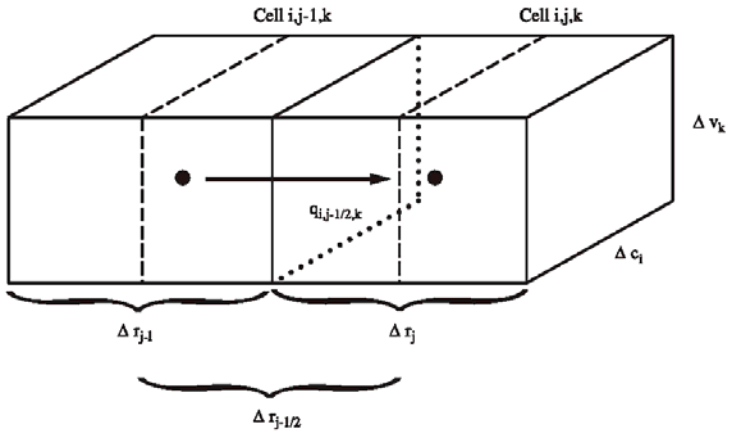

Figure 2–3. Flow into cell i,j,k from cell i,j-1,k. (Modified from McDonald and Harbaugh, 1988.)

Figure 2–2 depicts six aquifer cells adjacent to cell i,j,k — i-1,j,k; i+1,j,k; i,j-1,k; i,j+1,k; i,j,k-1; and i,j,k+1. To simplify the following development, flows are considered positive if they are entering cell i,j,k; the negative sign usually incorporated in Darcy's law has been dropped from all terms. Following these conventions, flow into cell i,j,k in the row direction from cell i,j-1,k (figure 2–3), is given by Darcy's law as

$$q_{i,j-1/2,k} = KR_{i,j-1/2,k}\Delta c_i \Delta v_k \frac{\left(h_{i,j-1,k} - h_{i,j,k}\right)}{\Delta r_{j-1/2}}, \qquad (2\text{–}3)$$

where

$h_{i,j,k}$ is the head at node i,j,k, and $h_{i,j-1,k}$ is the head at node i,j-1,k;

$q_{i,j-1/2,k}$ is the volumetric flow rate through the face between cells i,j,k and i,j-1,k (L^3T^{-1});

$KR_{i,j-1/2,k}$ is the hydraulic conductivity along the row between nodes i,j,k and i,j-1,k (LT^{-1});

$\Delta c_i \Delta v_k$ is the area of the cell faces normal to the row direction; and

$\Delta r_{j-1/2}$ is the distance between nodes i,j,k and i,j-1,k (L).

Equation 2–3 gives the exact flow for a one-dimensional steady-state case through a block of aquifer extending from node i,j-1,k to node i,j,k and having a cross-sectional area $\Delta c_i \Delta v_k$. KR i,j-1/2,k is the conductivity of the material between nodes i,j,k and i,j-1,k, which is the effective hydraulic conductivity for the entire region between the nodes, normally calculated as a harmonic mean in the sense described, for example, by Collins (1961).

The subscript i,j-1/2,k is used in equation 2–3 to designate the region between nodes i,j-1,k and i,j,k. The "1/2" does not indicate a specific point half way between nodes. Thus, $q_{i,j-1/2,k}$ indicates that the flow from node i,j-1,k to node i,j,k, $\Delta r_{j-1/2}$ is the distance between nodes i,j,k and i,j-1/2,k, and KR i,j-1/2,k is the effective hydraulic conductivity between the nodes. The term "1/2" is used in the same manner to indicate the region between nodes in many of the equations throughout this report.

Similar expressions can be written approximating the flow into the cell through the remaining five faces, for example, for flow in the row direction through the face between cells i,j,k and i,j+1,k,

$$q_{i,j+1/2,k} = KR_{i,j+1/2,k}\Delta c_i \Delta v_k \frac{\left(h_{i,j+1,k} - h_{i,j,k}\right)}{\Delta r_{j+1/2}}, \qquad (2\text{–}4)$$

while for the column direction, flow into the block through the front face is

$$q_{i+1/2,j,k} = KC_{i+1/2,j,k}\Delta r_j \Delta v_k \frac{\left(h_{i+1,j,k} - h_{i,j,k}\right)}{\Delta c_{i+1/2}} \tag{2–5}$$

and flow into the block through the rear face is

$$q_{i-1/2,j,k} = KC_{i-1/2,j,k}\Delta r_j \Delta v_k \frac{\left(h_{i-1,j,k} - h_{i,j,k}\right)}{\Delta c_{i-1/2}} . \tag{2–6}$$

For the vertical direction, inflow through the bottom face is

$$q_{i,j,k+1/2} = KV_{i,j,k+1/2}\Delta r_j \Delta c_i \frac{\left(h_{i,j,k+1} - h_{i,j,k}\right)}{\Delta v_{k+1/2}} , \tag{2–7}$$

whereas inflow through the upper face is given by

$$q_{i,j,k-1/2} = KV_{i,j,k-1/2}\Delta r_j \Delta c_i \frac{\left(h_{i,j,k-1} - h_{i,j,k}\right)}{\Delta v_{k-1/2}} . \tag{2–8}$$

Each of equations 2–3 through 2–8 expresses inflow through a face of cell i,j,k in terms of heads, grid dimensions, and hydraulic conductivity. The notation can be simplified by combining grid dimensions and hydraulic conductivity into a single constant, the "hydraulic conductance" or, more simply, the "conductance." For example,

$$CR_{i,j-1/2,k} = \frac{KR_{i,j-1/2,k}\Delta c_i \Delta v_k}{\Delta r_{j-1/2}} , \tag{2–9}$$

where

$CR_{i,j-1/2,k}$ is the conductance in row i and layer k between nodes i,j-1,k and i,j,k (L^2T^{-1}).

Thus, conductance is the product of hydraulic conductivity and cross-sectional area of flow divided by the length of the flow path (in this case, the distance between the nodes).

Substituting conductance from equation 2–9 into equation 2–3 yields

$$q_{i,j-1/2,k} = CR_{i,j-1/2,k}\left(h_{i,j-1,k} - h_{i,j,k}\right) . \tag{2–10}$$

Similarly, equations 2–4 through 2–8 can be rewritten to yield

$$q_{i,j+1/2,k} = CR_{i,j+1/2,k}\left(h_{i,j+1,k} - h_{i,j,k}\right) \tag{2–11}$$

$$q_{i-1/2,j,k} = CC_{i-1/2,j,k}\left(h_{i-1,j,k} - h_{i,j,k}\right) \tag{2–12}$$

$$q_{i+1/2,j,k} = CC_{i+1/2,j,k}\left(h_{i+1,j,k} - h_{i,j,k}\right) \tag{2–13}$$

$$q_{i,j,k-1/2} = CV_{i,j,k-1/2}\left(h_{i,j,k-1} - h_{i,j,k}\right) \tag{2–14}$$

$$q_{i,j,k+1/2} = CV_{i,j,k+1/2}\left(h_{i,j,k+1} - h_{i,j,k}\right) , \tag{2–15}$$

where the conductances are defined analogously to CR in equation (2–9).

Equations 2–10 through 2–15 account for the flow into cell i,j,k from the six adjacent cells. To account for flows into the cell from features or processes external to the aquifer, such as rivers, drains, areal recharge, evapotranspiration, or wells, additional terms are required. These flows may be dependent on the head in the receiving cell but independent of all other heads in the aquifer, or they may be entirely independent of the head in the receiving cell. Flow from outside the aquifer may be represented by the expression

$$a_{i,j,k,n} = p_{i,j,k,n} h_{i,j,k} + q_{i,j,k,n} \quad , \tag{2–16}$$

where

$a_{i,j,k,n}$ represents flow from the nth external source into cell i,j,k (L^3T^{-1}), and

$p_{i,j,k,n}$ and $q_{i,j,k,n}$ are constants ((L^2T^{-1}) and (L^3T^{-1}), respectively).

For example, suppose a cell is receiving flow from two sources, recharge from a well and seepage through a riverbed. For the first source (n=1), because the flow from the well is assumed to be independent of head, $p_{i,j,k,1}$ is zero and $q_{i,j,k,1}$ is the recharge rate for the well. In this case,

$$a_{i,j,k,1} = q_{i,j,k,1} \quad . \tag{2–17}$$

For the second source (n=2), the assumption is made that the river-aquifer interconnection can be treated as a simple conductance, so that the seepage is proportional to the head difference between the river stage and the head in cell i,j,k (figure 2–4); thus we have

$$a_{i,j,k,2} = \mathrm{CRIV}_{i,j,k}\left(R_{i,j,k} - h_{i,j,k}\right) \quad , \tag{2–18}$$

where

$R_{i,j,k}$ is the head in the river (L), and

$\mathrm{CRIV}_{i,j,k}$ is a conductance (L^2T^{-1}) controlling flow from the river into cell i,j,k.

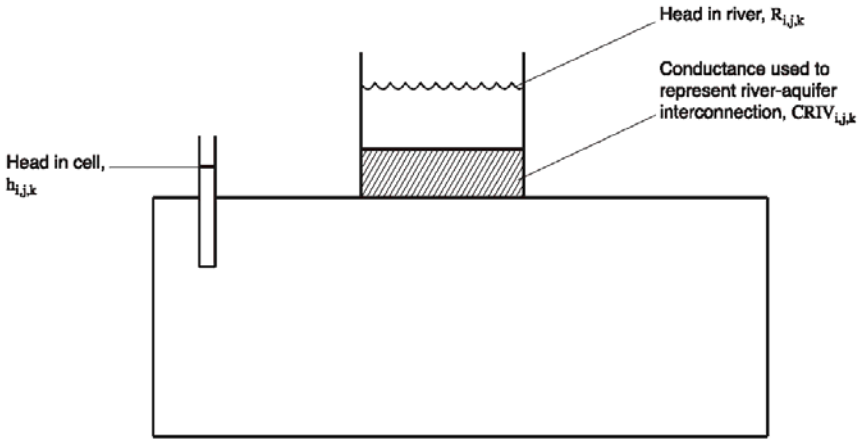

Figure 2–4. Conceptual representation of leakage through a riverbed into a cell. (Modified from McDonald and Harbaugh, 1988.)

For example, in the situation shown schematically in figure 2–4, CRIV would be given as the product of the vertical hydraulic conductivity of the riverbed material and the area of the riverbed as it crosses the cell, divided by the thickness of the riverbed material. Equation 2–18 can be rewritten as

$$a_{i,j,k,2} = -CRIV_{i,j,k} h_{i,j,k} + CRIV_{i,j,k} R_{i,j,k} \quad . \tag{2–19}$$

The negative conductance term, $-CRIV_{i,j,k}$ corresponds to $p_{i,j,k,2}$ of equation 2–16, while the term $CRIV_{i,j,k}R_{i,j,k}$ corresponds to $q_{i,j,k,2}$. Similarly, all other external sources or stresses can be represented by an expression of the form of equation 2–16. In general, if there are N external sources or stresses affecting a single cell, the combined flow is expressed by

$$\sum_{n=1}^{N} a_{i,j,k,n} = \sum_{n=1}^{N} \left(p_{i,j,k,n} h_{i,j,k} \right) + \sum_{n=1}^{N} q_{i,j,k,n} \quad . \tag{2–20}$$

Defining $P_{i,j,k}$ and $Q_{i,j,k}$ by the expressions

$$P_{i,j,k} = \sum_{n=1}^{N} p_{i,j,k,n}$$

and

$$Q_{i,j,k} = \sum_{n=1}^{N} q_{i,j,k,n}$$

the general external flow term for cell i,j,k is

$$\sum_{n=1}^{N} a_{i,j,k,n} = P_{i,j,k} h_{i,j,k} + Q_{i,j,k} \quad . \tag{2–21}$$

Applying the continuity equation 2–2 to cell i,j,k, taking into account the flows from the six adjacent cells, change in storage, and the external flow rate yields

$$\begin{aligned} & q_{i,j-1/2,k} + q_{i,j+1/2,k} + q_{i-1/2,j,k} + q_{i+1/2,j,k} \\ & + q_{i,j,k-1/2} + q_{i,j,k+1/2} + P_{i,j,k} h_{i,j,k} + Q_{i,j,k} = SS_{i,j,k} \left(\Delta r_j \Delta c_i \Delta v_k \right) \frac{\Delta h_{i,j,k}}{\Delta t} \quad , \end{aligned} \tag{2–22}$$

where

$\Delta h_{i,j,k}/\Delta t$ is a finite-difference approximation for the derivative of head with respect to time (LT^{-1});

$SS_{i,j,k}$ represents the specific storage of cell i,j,k (L^{-1}); and

$\Delta r_j \Delta c_i \Delta v_k$ is the volume of cell i,j,k (L^3).

Equations 2–10 through 2–15 may be substituted into equation 2–22 to give the finite-difference approximation for cell i,j,k as

$$\begin{aligned} & CR_{i,j-1/2,k} \left(h_{i,j-1,k} - h_{i,j,k} \right) + CR_{i,j+1/2,k} \left(h_{i,j+1,k} - h_{i,j,k} \right) \\ & + CC_{i-1/2,j,k} \left(h_{i-1,j,k} - h_{i,j,k} \right) + CC_{i+1/2,j,k} \left(h_{i+1,j,k} - h_{i,j,k} \right) \\ & + CV_{i,j,k-1/2} \left(h_{i,j,k-1} - h_{i,j,k} \right) + CV_{i,j,k+1/2} \left(h_{i,j,k+1} - h_{i,j,k} \right) \\ & + P_{i,j,k} h_{i,j,k} + Q_{i,j,k} = SS_{i,j,k} \left(\Delta r_j \Delta c_i \Delta v_k \right) \frac{\Delta h_{i,j,k}}{\Delta t} \quad . \end{aligned} \tag{2–23}$$

The finite-difference approximation for the time derivative of head, $\Delta h_{i,j,k}/\Delta t$ must next be expressed in terms of specific heads and times. Figure 2–5 shows a hydrograph of head values at node i,j,k. Two values of time are shown on the horizontal axis: t^m, the time at which the flow terms of equation (2–23) are evaluated; and t^{m-1}, a time that precedes t^m. The head values at node i,j,k associated with these times are designated by superscript as $h^m_{i,j,k}$ and $h^{m-1}_{i,j,k}$, respectively. An approximation to the time derivative of head at time t^m is obtained by dividing the head difference $h^m_{i,j,k} - h^{m-1}_{i,j,k}$ by the time interval $t^m - t^{m-1}$; that is,

$$\frac{\Delta h_{i,j,k}}{\Delta t} \cong \frac{h^m_{i,j,k} - h^{m-1}_{i,j,k}}{t^m - t^{m-1}} \quad .$$

Thus the hydrograph slope, or time derivative, is approximated using the change in head at the node over a time interval that precedes, and ends with, the time at which flow is evaluated. This is termed a backward-difference approach, in that $\Delta h/\Delta t$ is approximated over a time interval that extends backward in time from t^m, the time at which the flow terms are calculated.

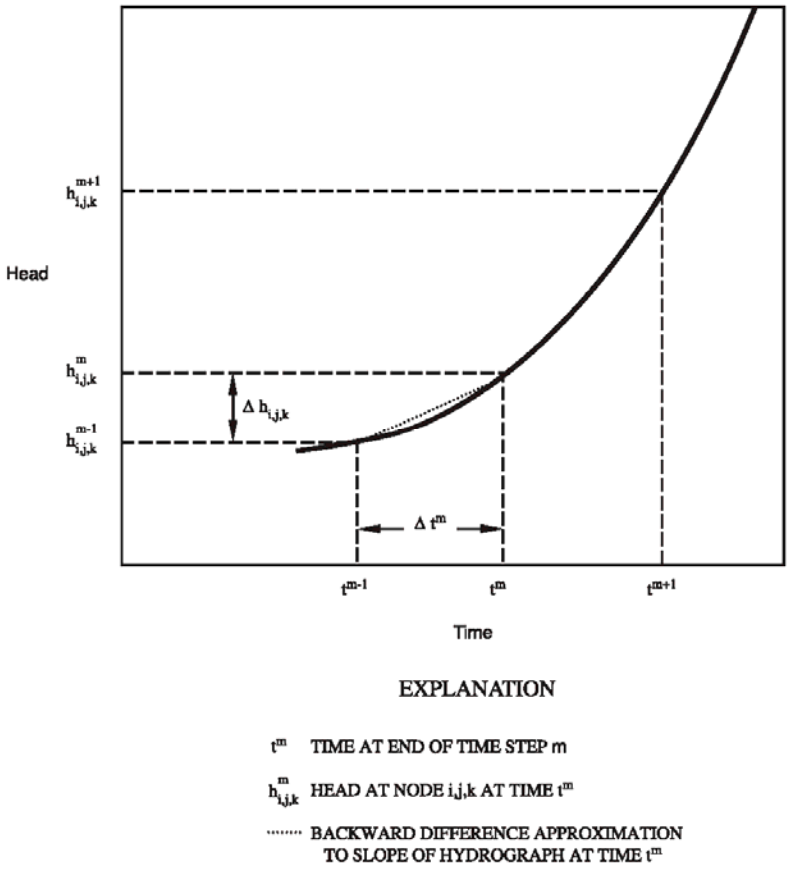

Figure 2–5. Hydrograph for cell i,j,k. (Modified from McDonald and Harbaugh, 1988.)

The time derivative of head could be approximated in other ways; for example, we could approximate the time derivative of head over a time interval that begins at the time of flow evaluation and extends to some later time; or over a time interval that is centered at the time of flow evaluation, extending both forward and backward from it. These alternatives, however, may cause numerical instability—that is, the growth or propagation of error during the calculation of heads at successive times in a simulation. In an unstable situation, errors that enter the calculation for any reason at a particular time will increase at each succeeding time as the calculation progresses, until finally the errors completely dominate the result. By contrast, the backward-difference approach is always numerically stable—that is, errors introduced at any time diminish progressively at succeeding times. For this reason, the

backward-difference approach is preferred even though this approach leads to large systems of equations that must be solved simultaneously for each time step.

Equation 2–23 can be rewritten in backward-difference form by specifying flow terms at t^m, the end of the time interval, and approximating the time derivative of head over the interval t^{m-1} to t^m; that is:

$$\begin{aligned} & CR_{i,j-1/2,k}\left(h^m_{i,j-1,k} - h^m_{i,j,k}\right) + CR_{i,j+1/2,k}\left(h^m_{i,j+1,k} - h^m_{i,j,k}\right) \\ & + CC_{i-1/2,j,k}\left(h^m_{i-1,j,k} - h^m_{i,j,k}\right) + CC_{i+1/2,j,k}\left(h^m_{i+1,j,k} - h^m_{i,j,k}\right) \\ & + CV_{i,j,k-1/2}\left(h^m_{i,j,k-1} - h^m_{i,j,k}\right) + CV_{i,j,k+1/2}\left(h^m_{i,j,k+1} - h^m_{i,j,k}\right) \\ & + P_{i,j,k}h^m_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}\left(\Delta r_j \Delta c_i \Delta v_k\right)\frac{h^m_{i,j,k} - h^{m-1}_{i,j,k}}{t^m - t^{m-1}} \ . \end{aligned} \tag{2–24}$$

Equation 2–24 is a backward-difference equation that can be used as the basis for a simulation of the partial-differential equation of ground-water flow, equation 2–1. Like the term $Q_{i,j,k}$, the coefficients of the various head terms in equation 2–24 are all known, as is the head at the beginning of the time step, $h^{m-1}_{i,j,k}$. The seven heads at time t^m, the end of the time step, are unknown; that is, they are part of the head distribution to be predicted. Thus equation 2–24 cannot be solved independently, because it represents a single equation in seven unknowns. An equation of this type, however, can be written for each active cell in the grid; and, because only one unknown head exists for each cell, we are left with a system of "n" equations in "n" unknowns. Such a system can be solved simultaneously.

The objective of transient simulation is generally to predict head distributions at successive times, given the initial head distribution, the boundary conditions, the hydraulic parameters, and the external stresses. The initial-head distribution provides a value of $h^0_{i,j,k}$ at each point in the grid—that is, the initial head provides the values of head at the beginning of the first of the discrete time steps into which the time axis is divided in the finite-difference process. The first step in the solution process is to calculate values of $h^1_{i,j,k}$—that is, heads at time t^1, which marks the end of the first time step. In equation 2–24, therefore, the head superscript m is taken as 1, while the superscript m-1, which appears in only one head term, is taken as 0. Equation 2–24 then becomes

$$\begin{aligned} & CR_{i,j-1/2,k}\left(h^1_{i,j-1,k} - h^1_{i,j,k}\right) + CR_{i,j+1/2,k}\left(h^1_{i,j+1,k} - h^1_{i,j,k}\right) \\ & + CC_{i-1/2,j,k}\left(h^1_{i-1,j,k} - h^1_{i,j,k}\right) + CC_{i+1/2,j,k}\left(h^1_{i+1,j,k} - h^1_{i,j,k}\right) \\ & + CV_{i,j,k-1/2}\left(h^1_{i,j,k-1} - h^1_{i,j,k}\right) + CV_{i,j,k+1/2}\left(h^1_{i,j,k+1} - h^1_{i,j,k}\right) \\ & + P_{i,j,k}h^1_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}\left(\Delta r_j \Delta c_i \Delta v_k\right)\frac{h^1_{i,j,k} - h^0_{i,j,k}}{t^1 - t^0} \ , \end{aligned} \tag{2–25}$$

where again, the superscripts 0 and 1 refer to the time at which the heads are taken and should not be interpreted as exponents.

An equation of this form is written for every cell in the grid in which head is free to vary with time (variable-head cells), and the system of equations is solved simultaneously for the heads at time t^1. When these have been obtained, the process is repeated to obtain heads at time t^2, the end of the second time step. To do this, equation 2–24 is reapplied, now using 1 as time superscript m-1 and 2 as time superscript m. Again, a system of equations is formulated, where the unknowns are now the heads at time t^2; and this set of equations is solved simultaneously to obtain the head distribution at time t^2. This process is continued for as many time steps as necessary to cover the time range of interest.

The set of finite-difference equations is reformulated at each time step; that is, at each time step there is a new system of simultaneous equations to be solved. The heads at the end of the time step make up the unknowns for which this system must be solved; the heads at the beginning of the step are among the known terms in the equations. The solution process is repeated at each time step yielding a new array of heads for the end of the step.

The finite-difference flow equation for a cell is a representation of the volumetric flow from all sources in units of L^3/T, where L is a length unit and T is a time unit. Provided that consistent length and time units are used for all terms, any specific units can be used. For example, length units could be feet and time units could be days, or length units could be meters and time units could be seconds. This gives a certain amount of freedom to the user, but care must be exercised to avoid mixing units when specifying the input data. The use of inconsistent units cannot be detected. For example, if conductance is specified in units of square feet per day and an external recharge rate is given in units of cubic meters per second, the resulting flow equation will be meaningless.

Iteration

MODFLOW utilizes iterative methods to obtain the solution to the system of finite-difference equations for each time step. In these methods, the calculation of head values for the end of a given time step is started by arbitrarily assigning a trial value, or estimate, for the head at each node at the end of that step. A procedure of calculation is then initiated that alters these estimated values, producing a new set of head values that are in closer agreement with the system of equations. These new, or interim, head values then take the place of the initially assumed heads, and the procedure of calculation is repeated, producing a third set of head values. This procedure is repeated successively at each stage, producing a new set of interim heads that more nearly satisfies the system of equations. Each repetition of the calculation is termed an "iteration." Ultimately, as the interim heads approach values that would exactly satisfy the set of equations, the changes produced by succeeding stages of calculation become very small. This behavior is utilized in determining when to stop iteration, as discussed in a subsequent paragraph.

Thus, during the calculations for a time step, arrays of interim head values are generated in succession, each array containing one interim head value for each active node in the grid. In figure 2–6, these arrays are represented as three-dimensional lattices, each identified by an array symbol, h, bearing two superscripts. The first superscript indicates the time step for which the heads in the array are calculated, whereas the second indicates the number, or level, of the iteration that produced the head array. Thus $h^{m,1}$ represents the array of values computed in the first iteration for time step m; $h^{m,2}$ would represent the array of values computed in the second iteration, and so on. The head values that were initially assumed for time step m, to begin the process of iteration, appear in the array designated $h^{m,0}$. In the example of figure 2–6, a total of n iterations is required to achieve closure for the heads at the end of time step m; thus the array of final head values for the time step is designated $h^{m,n}$. Figure 2–6 also shows the array of final head values for the end of the preceding time step $h^{m-1,n}$ (where again it is assumed that n iterations were required for closure). The head values in this array appear in the storage term of equation 2–24—that is, they are used in the term $h_{i,j,k}^{m-1}$ on the right side of equation 2–24—in the calculation of heads for time step m. Because they represent heads for the preceding time step, for which computations have already been completed, they appear as predetermined constants in the equation for time step m; thus they retain the same value in each iteration of the time step. Similarly, the final values of head for time step m are used as constants in the storage term during calculations for time step m+1.

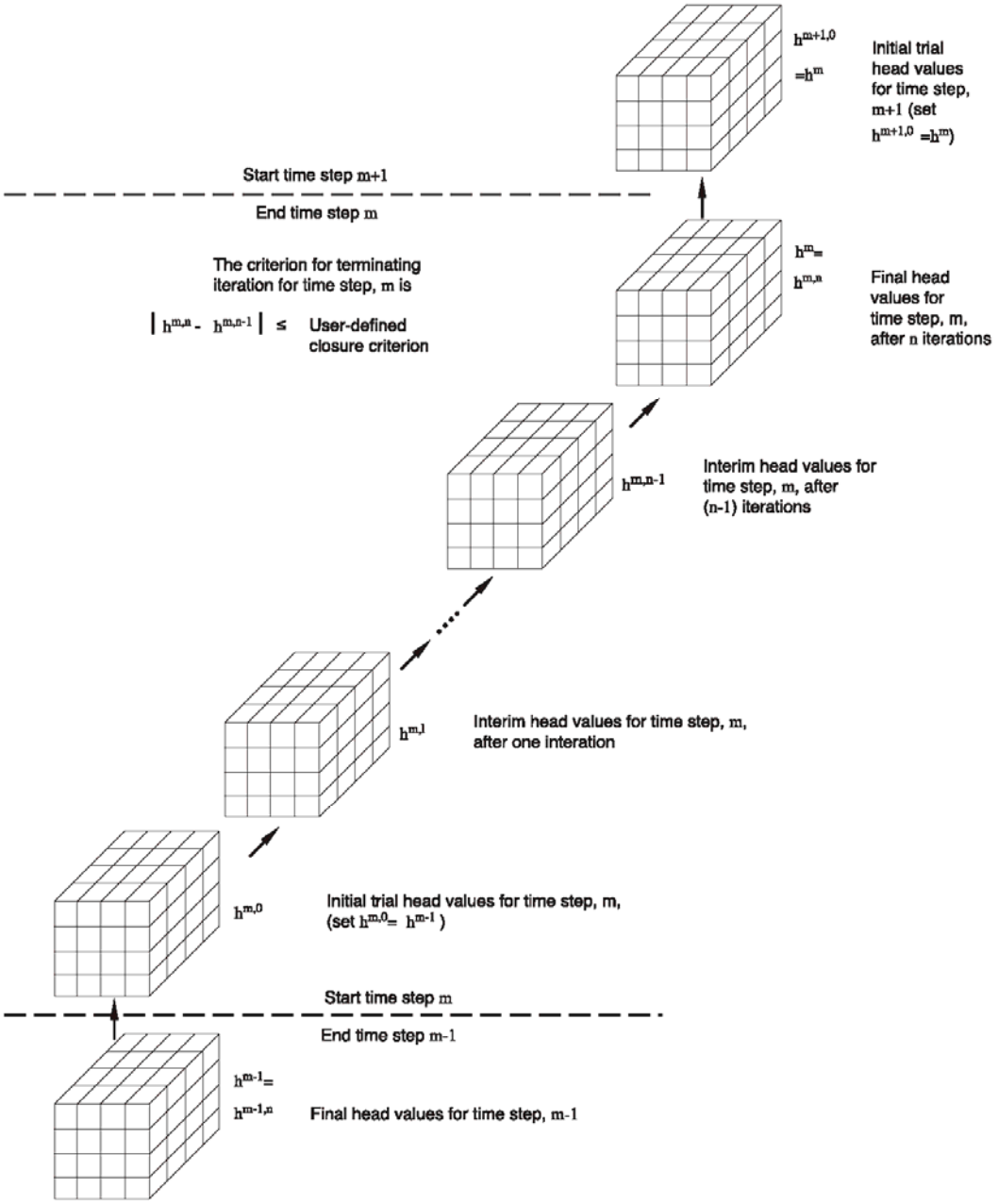

Figure 2–6. Iterative calculation of a head distribution. (From McDonald and Harbaugh, 1988.)

Ideally, one would like to specify that iteration stop when the calculated heads are suitably close to the exact solution. Because the actual solution is unknown, however, an indirect method of specifying when to stop iterating must be used. The method most commonly employed is to specify that the changes in computed heads occurring from one iteration level to the next must be less than a certain quantity, termed the "closure criterion" or "convergence criterion," which is specified by the user. After each iteration, absolute values of computed head change in that iteration are examined for all nodes in the grid. The largest of these absolute head-change values is compared with the closure criterion. If this largest value exceeds the closure criterion, iteration continues; if this value is less than the closure criterion, iteration is said to have "closed" or "converged," and the process is terminated for that time step. Normally, this method of determining when to stop iteration is adequate. Note that the closure criterion refers to change in computed head, and that values of head are not themselves necessarily calculated to a level of accuracy comparable to the closure criterion. As a rule of thumb, it is wise to use a value of closure criterion that is an order of magnitude smaller than the level of accuracy desired in the head results.

MODFLOW also incorporates a maximum permissible number of iterations per time step. If closure is not achieved within this maximum number of iterations, then the iterative process is terminated and a corresponding message is printed in the output.

The initial estimates of head for time step m, in array $h^{m,0}$ of figure 2–6, could be assigned arbitrarily, or they could be chosen according to a number of different conventions. Theoretically, the iterative process would eventually converge to the same result regardless of the choice of initial head values, although the work required would be much greater for some choices than for others. In MODFLOW, the heads computed for the end of each time step are used as the initial trial values of head for the succeeding time step. Thus in figure 2–6, the array $h^{m-1,n}$ contains the final estimates of head, obtained after n iterations, for the end of time step m-1. When the calculations for step m-1 are complete, these same values of head are transferred to the array $h^{m,0}$, and used as the initial estimates, or trial values, for the heads of time step m. Head values for the first time step in the simulation are assumed initially to be equal to the heads specified by the user for the beginning of the simulation.

Discussions of the mathematical basis of various iterative methods can be found in many standard references, including Peaceman (1977), Crichlow (1977) and Remson, Hornberger and Molz (1971). The reader is advised to review one of these discussions, both to clarify general concepts and to provide an introduction to such topics as the use of matrix notation, the role of iteration parameters, and the influence of various factors on rate of convergence. In particular, such a review is recommended prior to reading Chapter 7 of this report.

An iterative procedure yields only an approximation to the solution of the system of finite-difference equations for each time step; the accuracy of this approximation depends upon several factors, including the closure criterion that is employed. Even if exact solutions to the set of finite-difference equations were obtained at each step, these solutions would themselves be only an approximation to the solution of the differential equation of flow (eq. 2–1). The discrepancy between the head, $h^{m}_{i,j,k}$, given by the solution to the system of difference equations for a given node and time and the head h(x,y,z,t), which would be given by the formal solution of the differential equation for the corresponding point and time, is termed the truncation error. In general, this error tends to become greater as the grid spacing and time-step length are increased. The reader also should recognize that even if a formal solution of the differential equation could be obtained, it would be only an approximation to conditions in the field, in that hydraulic conductivity and specific storage are seldom known with accuracy, and uncertainties with regard to hydrologic boundaries are generally present.

Steady-State Simulations

The flow equation, equation 2–24, was developed assuming transient conditions; however, the transient flow equation becomes the steady-state flow equation when the storage term is zero. The resulting equation specifies that the sum of all inflows (where outflow is a negative inflow) from adjacent cells and external stresses must be zero for each cell in the model. A steady-state problem requires only a single solution of simultaneous equations, rather than multiple solutions for multiple time steps. Recall that an initial head was required in a transient simulation to calculate the time derivative for the first time step. For steady-state simulations, there is no direct requirement for initial head because the time derivative is removed from the flow equation. In practice, however, initial head is required for steady-state simulations because of the assumption that iterative solution is used. As already described, iterative solution works by successively improving the estimated answer; therefore, an initial estimate is required to start the iterative process. In MODFLOW, the user-specified initial head is used as this initial estimate. The initial estimate should normally have no effect on the solution to the steady-state flow equation, but it may affect the number of iterations required to obtain an acceptable approximation of the solution.

Formulation of Equations for Solution

MODFLOW incorporates several different options for iterative solution of the set of finite-difference equations, and is organized so that alternative schemes of solution may be added without disruption of the program structure. Whatever scheme of solution is employed, it is convenient to rearrange equation 2–24 so that all terms containing heads at the end of the current time step are grouped on the left-hand side of the equation, and all terms that are independent of head at the end of the current time step are on the right-hand side. All coefficients of $h^{m}_{i,j,k}$ that do not include conductance between nodes are combined into a single term, HCOF, and all right-hand-side terms are

combined into the term RHS. Further, the complexity can be reduced by assuming that the time superscript is m unless otherwise shown. The resulting equation is

$$\begin{aligned} &CV_{i,j,k-1/2}\,h_{i,j,k-1} + CC_{i-1/2,j,k}\,h_{i-1,j,k} + CR_{i,j-1/2,k}\,h_{i,j-1,k} \\ &+ (-CV_{i,j,k-1/2} - CC_{i-1/2,j,k} - CR_{i,j-1/2,k} - CR_{i,j+1/2,k} - CC_{i+1/2,j,k} - CV_{i,j,k+1/2} + HCOF_{i,j,k})\,h_{i,j,k} \\ &+ CR_{i,j+1/2,k}\,h_{i,j+1,k} + CC_{i+1/2,j,k}\,h_{i+1,j,k} + CV_{i,j,k+1/2}\,h_{i,j,k+1} = RHS_{i,j,k}\ , \end{aligned} \qquad (2\text{–}26)$$

where

$$HCOF_{i,j,k} = P_{i,j,k} - \frac{SS_{i,j,k}\,\Delta r_j\,\Delta c_i\,\Delta v_k}{t - t^{m-1}} \qquad (L^2T^{-1}) \text{ and}$$

$$RHS_{i,j,k} = -Q_{i,j,k} - SS_{i,j,k}\,\Delta r_j\,\Delta c_i\,\Delta v_k \frac{h_{i,j,k}^{m-1}}{t - t^{m-1}} \qquad (L^3T^{-1}).$$

The entire system of equations of the form of equation 2–26, which includes one equation for each variable-head cell in the grid, may be written in matrix form as

$$[A]\{h\} = \{q\}\ , \qquad (2\text{–}27)$$

where

[A] is a matrix of the coefficients of head, from the left side of equation 2–26, for all active nodes in the grid;

{h} is a vector of head values at the end of time step m for all nodes in the grid; and

{q} is a vector of the constant terms, RHS, for all nodes of the grid.

MODFLOW assembles the vector {q} and the terms that comprise [A] through a series of subroutines. The vector {q} and the terms comprising [A] are then transferred to subroutines that actually solve the matrix equations for the vector {h}.

Types of Model Cells and Simulation of Boundaries

In practice, formulating an equation of the form of equation 2–24 for every cell in a model grid is generally unnecessary, because the status of certain cells is specified in advance to simulate the boundary conditions of the problem. In MODFLOW, cells used to simulate boundary conditions are grouped into two categories—"constant-head" cells and "no-flow" cells. Constant-head cells are those for which the head is specified for each time, and the head value does not change as a result of solving the flow equations. No-flow cells are those for which no flow into or out of the cell is permitted. The remaining cells of the grid, termed "variable-head" cells in this report, are characterized by heads that are unspecified and free to vary with time. An equation of the form of equation 2–24 must be formulated for each variable-head cell in the grid, and the resulting system of equations must be solved simultaneously for each time step in the simulation.

Constant-head and no-flow cells are used in MODFLOW to represent conditions along various hydrologic boundaries inside the grid. For example, figure 2–7 shows the map of an aquifer boundary superimposed onto a grid of cells generated for the model. The aquifer is of irregular shape, whereas the model grid is always rectangular in outline. In areas where the aquifer is coincident with the outside edge of the grid, no special designation is needed to indicate no flow because MODFLOW does not compute inter-cell flow through the outside edges of the grid, including the top and bottom. Within the grid, no-flow cells have been used to delete the part of the grid beyond the aquifer boundary. The figure also shows constant-head cells along one section of the boundary; these may be used, for example, where the aquifer is in direct contact with major surface-water features. Other boundary conditions, such as areas of constant inflow or areas where inflow varies with head, can be simulated through the use of external source terms (Chapter 6) or through a combination of no-flow cells and external source terms. If flow occurs to or

from the outside of the grid where the aquifer extends to edge of the grid, then the flow can be simulated by using external source terms in the cells at the edges of the grid.

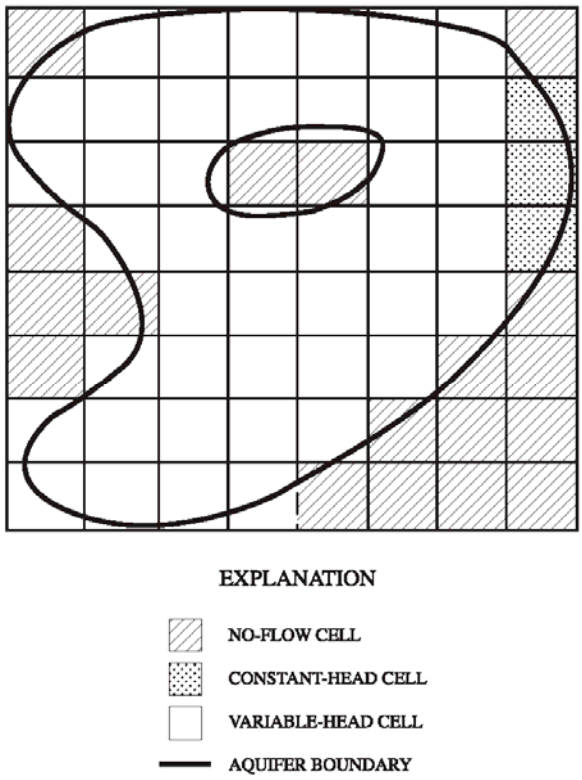

Figure 2–7. Discretized aquifer showing boundaries and cell designations. (Modified from McDonald and Harbaugh, 1988.)

Conceptual Aspects of Vertical Discretization

MODFLOW handles discretization of space in the horizontal direction by reading the number of rows, the number of columns, and the width of each row and column (that is, the width of the cells in the direction transverse to the row or column). Discretization of space in the vertical direction is handled in the model by specifying the number of layers to be used, and by specifying the top and bottom elevations of every cell in each layer.

At one extreme, vertical discretization can be visualized simply as an extension of areal discretization—a more or less arbitrary process of dividing the flow system into segments in the vertical dimension, governed in part by the vertical resolution desired in the results. At the opposite extreme, vertical discretization can be viewed as an effort to represent individual aquifers or permeable zones by individual layers of the model. Figure 2–8A shows a typical geohydrologic sequence that has been discretized in figures 2–8B and 2–8C according to both interpretations. The first viewpoint (fig. 2–8B) leads to rigid superposition of an orthogonal three-dimensional grid on the geohydrologic system; while there may be a general correspondence between geohydrologic layers and model layers, no attempt is made to make the grid conform to stratigraphic irregularities. Under the second viewpoint (fig. 2–8C), model layer thickness is considered variable, to simulate the varying thickness of geohydrologic units; this leads, in effect, to a deformed grid.

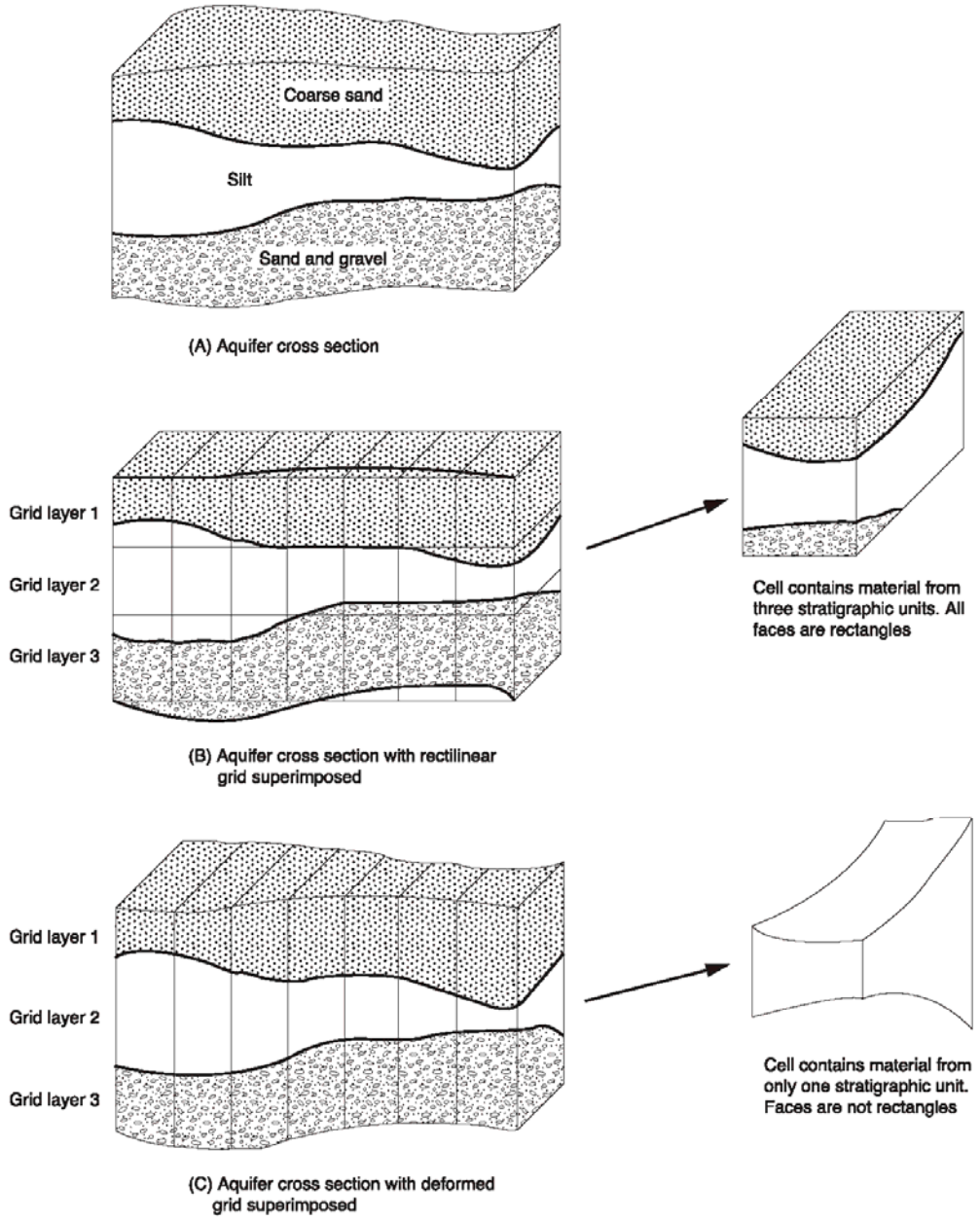

Figure 2–8. Schemes of vertical discretization. (From McDonald and Harbaugh, 1988.)

Each of these methods of viewing the vertical discretization process has advantages, and each presents difficulties. The model equations are based on the assumption that hydraulic properties are uniform within individual cells, or at least that meaningful average or integrated properties can be specified for each cell; these conditions are more likely to be met when model layers conform to geohydrologic units as in figure 2–8C. Moreover, greater accuracy can be expected if model layers correspond to intervals within which vertical head loss is negligible, and this is also more likely under the configuration of 2–8C. On the other hand, the deformed grid of 2–8C fails to conform to many of the assumptions upon which the model equations are based; for example, individual cells no longer have rectangular faces, and the major axes of hydraulic conductivity may not be aligned with the model grid. Some error is always introduced by these departures from assumed conditions.

In practice, many vertical discretization schemes turn out to be a combination of the viewpoints illustrated in figures 2–8B and 2–8C. For example, even where layer boundaries conform to geohydrologic contacts, the use of more than one layer to simulate a single geohydrologic unit may be necessary simply to achieve the required model

accuracy. Figure 2–9 shows a system consisting of two sand units separated by a clay unit; the units are of uniform thickness, and each could be represented by a single layer without deformation of the grid. However, head at each horizontal location would be represented by a single value in each unit; if greater detail in representing the vertical head distribution in the units is required, multiple layers must be used to represent each unit. Similarly, figure 2–10 shows a sand-clay system in which pumpage from the sands is sustained partially by vertical flow of water released from storage in the clay. If the objective of analysis is to determine the pattern of storage release in the clay, several model layers would be required to represent that unit, as shown in the figure. On the other hand, figure 2–11 shows a sand-clay system in which storage release occurs only in the sands, flow in the sand is essentially horizontal, and flow in the clay is essentially vertical. In this case, a single model layer may be used to represent each sand unit, whereas the clay may be represented simply by the vertical conductance between layers. This approach to vertical discretization has been termed the "Quasi Three-Dimensional" approach.

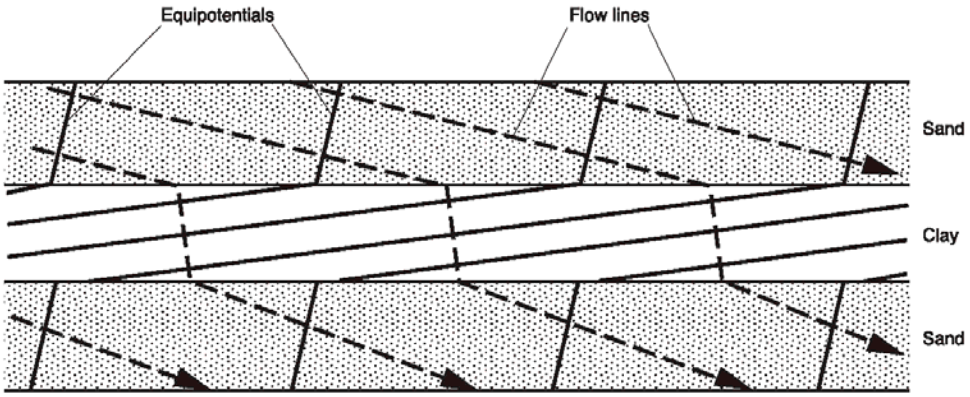

Figure 2–9. Possible pattern of flow in a cross section consisting of two high-conductivity units separated by a low-conductivity unit. (From McDonald and Harbaugh, 1988.)

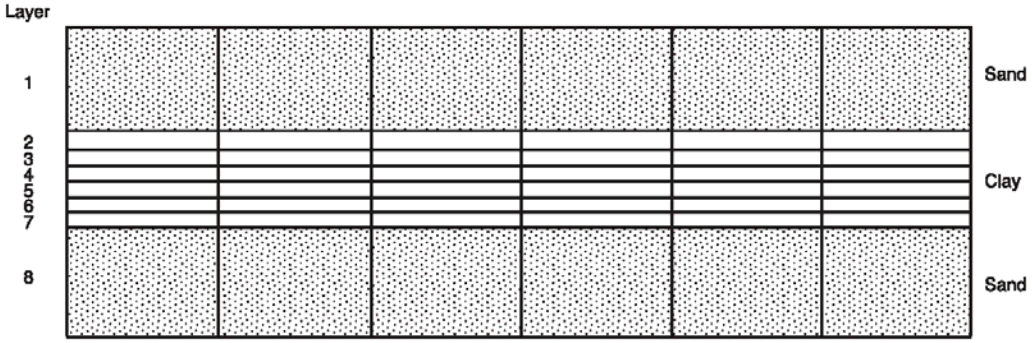

Figure 2–10. A cross section in which a low-conductivity unit is represented by six model layers. (Modified from McDonald and Harbaugh, 1988.)

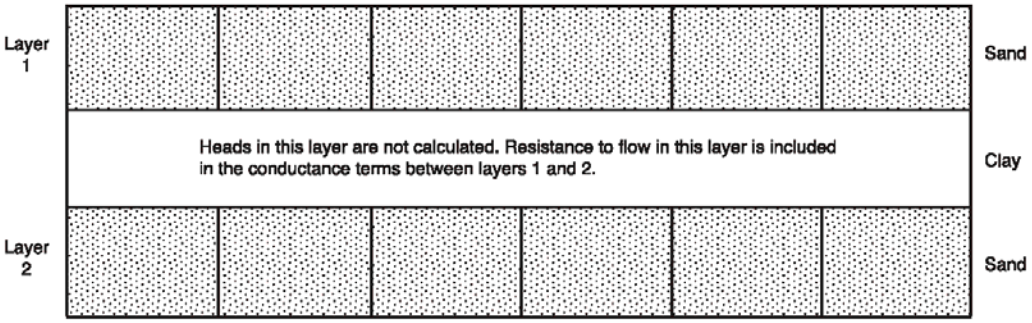

Figure 2–11. A cross section in which a low-conductivity unit is represented by the conductance between model layers. (From McDonald and Harbaugh, 1988.)

The approaches to vertical discretization described above all lead to a set of equations of the form of equation 2–26, which must be solved simultaneously at each time step. The differences among these approaches arise in the way the various conductances and storage terms are formulated and, in general, in the number of equations to be solved, the resolution of the results, and the accuracy of the results. MODFLOW is capable of implementing any of these approaches to vertical discretization in that the elevations of the individual cells in each layer can vary. Chapter 5, which describes the Block-Centered Flow and Layer-Property Flow Packages, contains a discussion of the formulation of conductance and storage terms corresponding to the various ways of conceptualizing the vertical discretization.