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

Chapter A1

A MODULAR THREE-DIMENSIONAL FINITE-DIFFERENCE GROUND-WATER FLOW MODEL

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Book 6

MODELING TECHNIQUES

Within each cell there is a point called a "node" at which head is to be calculated. Figure 2 illustrates, in two dimensions, two conventions for defining the configuration of cells with respect to the location of nodes--the block-centered formulation and the point-centered formulation. Both systems start by dividing the aquifer with two sets of parallel lines which are orthogonal. In the block-centered formulation, the blocks formed by the sets of parallel lines are the cells; the nodes are at the center of the cells. In the point-centered formulation, the nodes are at the intersection points of the sets of parallel lines, and cells are drawn around the nodes with faces halfway between nodes. In either case, spacing of nodes should be chosen so that the hydraulic properties of the system are, in fact, generally uniform over the extent of a cell. The finite-difference equation developed in the following section holds for either formulation; however, only the block-centered formulation is presently used in the model.

In equation (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.

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

$$\Sigma Q_i = SS\frac{\Delta h}{\Delta t}\Delta V \qquad (2)$$

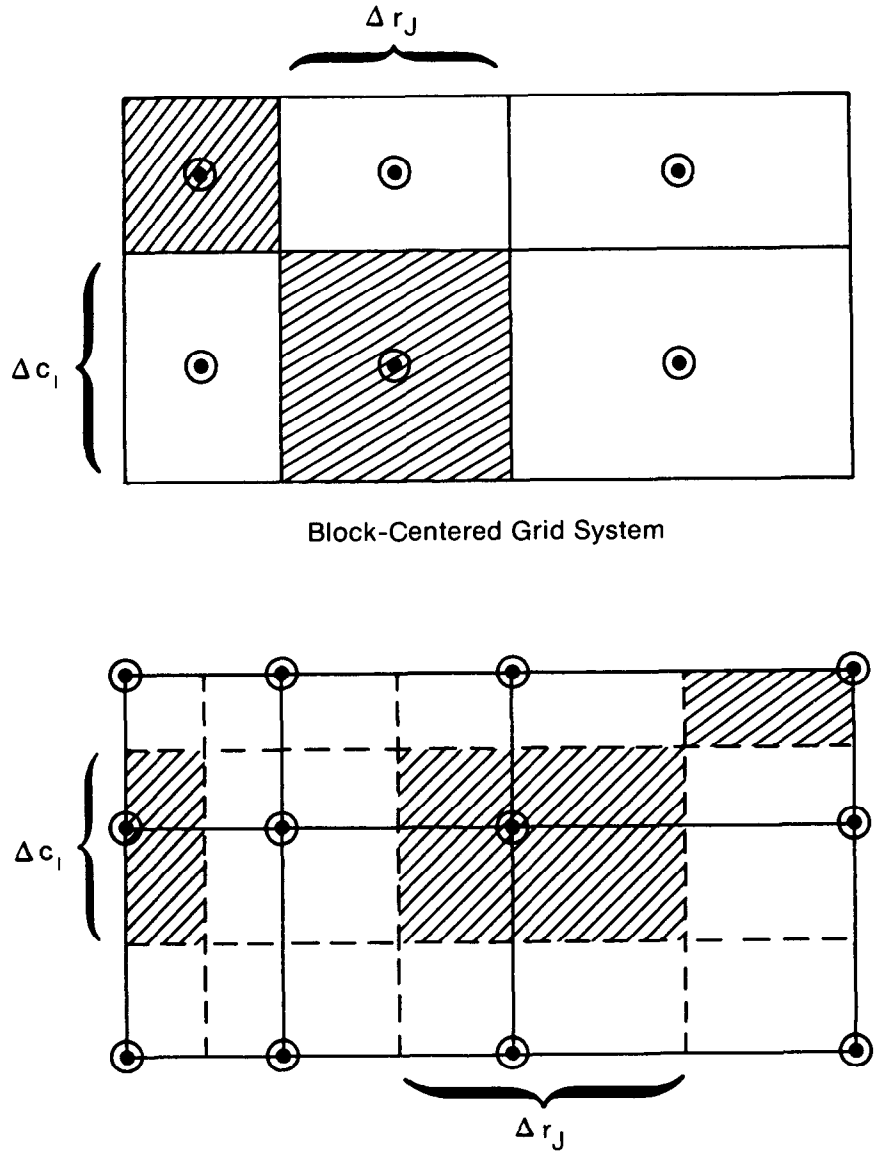


Figure 2.—Grids showing the difference between block-centered and point-centered grids.

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 (1)--i.e., it is the volume of water which 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) 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 3 depicts a cell i,j,k and six adjacent aquifer cells 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; and 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 4), is given by Darcy's law as

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

where

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

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

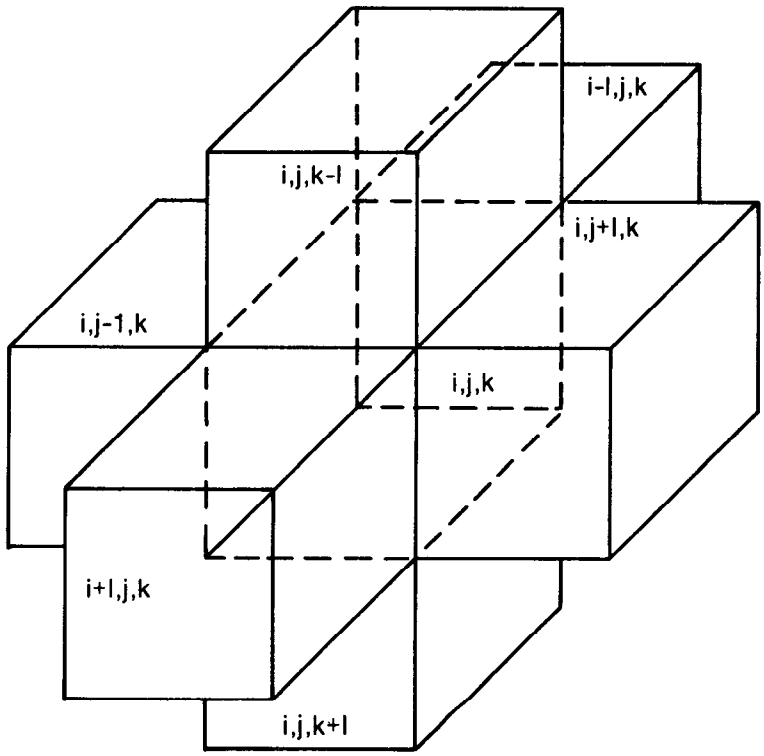


Figure 3.—Cell i,j,k and indices for the six adjacent cells.

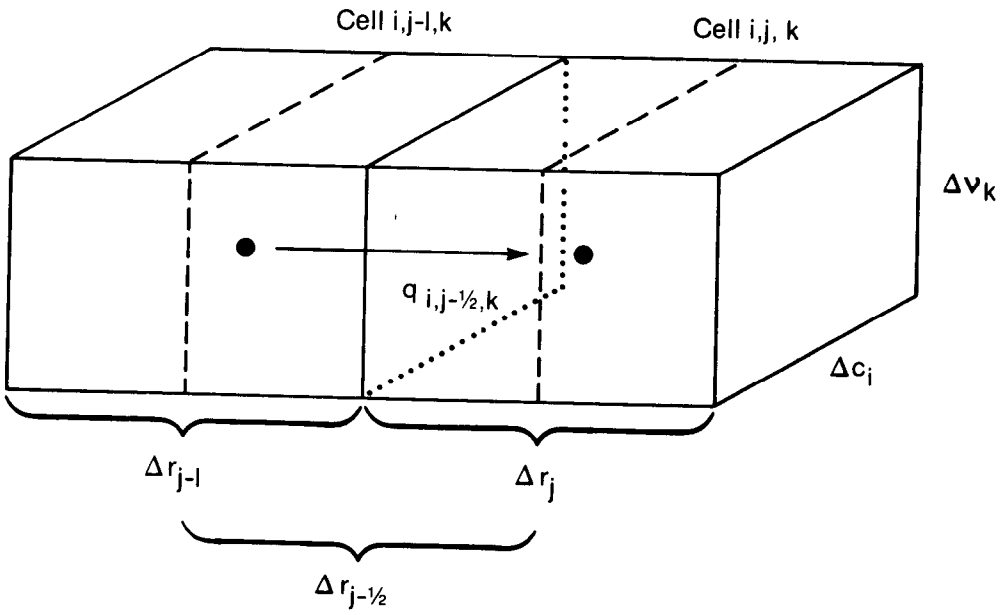


Figure 4.—Flow into cell i,j,k from cell i,j-l,k.

$KR_{i,j-1/2,k}$ 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).

Although the discussion is phrased in terms of flow into the central cell, it can be misleading to associate the subscript j-1/2 of equation (3) with a specific point between the nodes. Rather, the term $KR_{i,j-1/2,k}$ of equation (3) is the effective hydraulic conductivity for the entire region between the nodes, normally calculated as a harmonic mean in the sense described by, for example, Collins (1961). If this is done, equation (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 $\Delta c_i \Delta v_k$.

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

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

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

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

and flow into the block through the rear face is

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

For the vertical direction, inflow through the bottom face is

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

while inflow through the upper face is given by

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

Each of equations (3)-(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,

$$CR_{i,j-1/2,k} = KR_{i,j-1/2,k}\,\Delta c_i \Delta v_k / \Delta r_{j-1/2} \qquad (9)$$

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}).

Conductance is thus 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 (9) into equation (3) yields

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

Similarly, equations (4)-(8) can be rewritten to yield

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

$$q_{i-1/2,j,k} = CC_{i-1/2,j,k}(h_{i-1,j,k} - h_{i,j,k}) \quad (12)$$

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

$$q_{i,j,k-1/2} = CV_{i,j,k-1/2}(h_{i,j,k-1} - h_{i,j,k}) \quad (14)$$

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

where the conductances are defined analogously to $CR_{i,j-1/2,k}$ in equation (9).

Equations (10)-(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 streams, 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 head in the receiving cell. Flow from outside the aquifer may be represented by the expression

$$a_{i,j,k,n} = p_{i,j,k,n}h_{i,j,k} + q_{i,j,k,n} \quad (16)$$

where

$a_{i,j,k,n}$ represents flow from the n^{th} 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),

since 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,

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

For the second source (n=2), the assumption is made that the stream-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 5); thus we have

$$a_{i,j,k,2} = CRIV_{i,j,k,2}(R_{i,j,k} - h_{i,j,k}) \tag{18}$$

where $R_{i,j,k}$ is the head in the river (L) and $CRIV_{i,j,k,2}$ is a conductance (L^2t^{-1}) controlling flow from the river into cell i,j,k. For example, in the situation shown schematically in figure 5, CRIV would be given as the product of the vertical hydraulic conductivity of the riverbed material and the area of the streambed as it crosses the cell, divided by the thickness of the streambed material. Equation (18) can be rewritten as

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

The negative conductance term, $-CRIV_{i,j,k,2}$ corresponds to $p_{i,j,k,2}$ of equation 16, while the term $CRIV_{i,j,k,2}R_{i,j,k}$ 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 16. In general, if there are N external sources or stresses affecting a single cell, the combined flow is expressed by

$$QS_{i,j,k} = \sum_{n=1}^{N} a_{i,j,k,n} = \sum_{n=1}^{N} p_{i,j,k,n}\ h_{i,j,k} + \sum_{n=1}^{N} q_{i,j,k,n}. \tag{20}$$

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

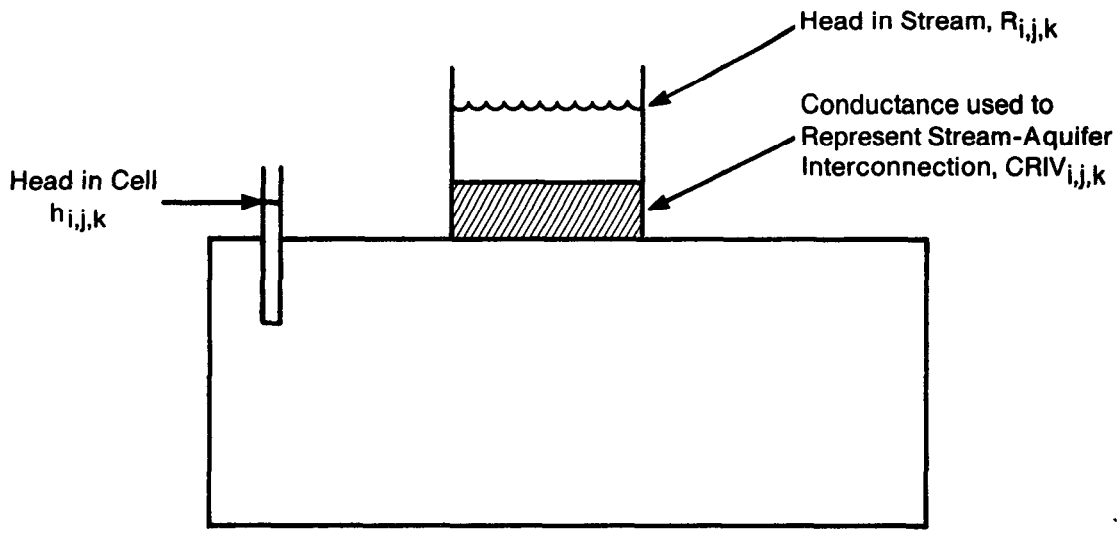


Figure 5.—Conceptual representation of leakage through a riverbed into a cell.

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

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

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

$$QS_{i,j,k} = P_{i,j,k}h_{i,j,k} + Q_{i,j,k}. \tag{21}$$

Applying the continuity equation (2) to cell i,j,k, taking into account the flows from the six adjacent cells, as well as the external flow rate, QS, yields

$$q_{i,j-1/2,k} + q_{i,j+1/2,k} + q_{i-1/2,j,k} + q_{i+1/2,j,k}$$

$$+ q_{i,j,k-1/2} + q_{i,j,k+1/2} + QS_{i,j,k} = SS_{i,j,k}\frac{\Delta h_{i,j,k}}{\Delta t}\Delta r_j \Delta c_i \Delta v_k \tag{22}$$

where

$\frac{\Delta h_{i,j,k}}{\Delta t}$ 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).

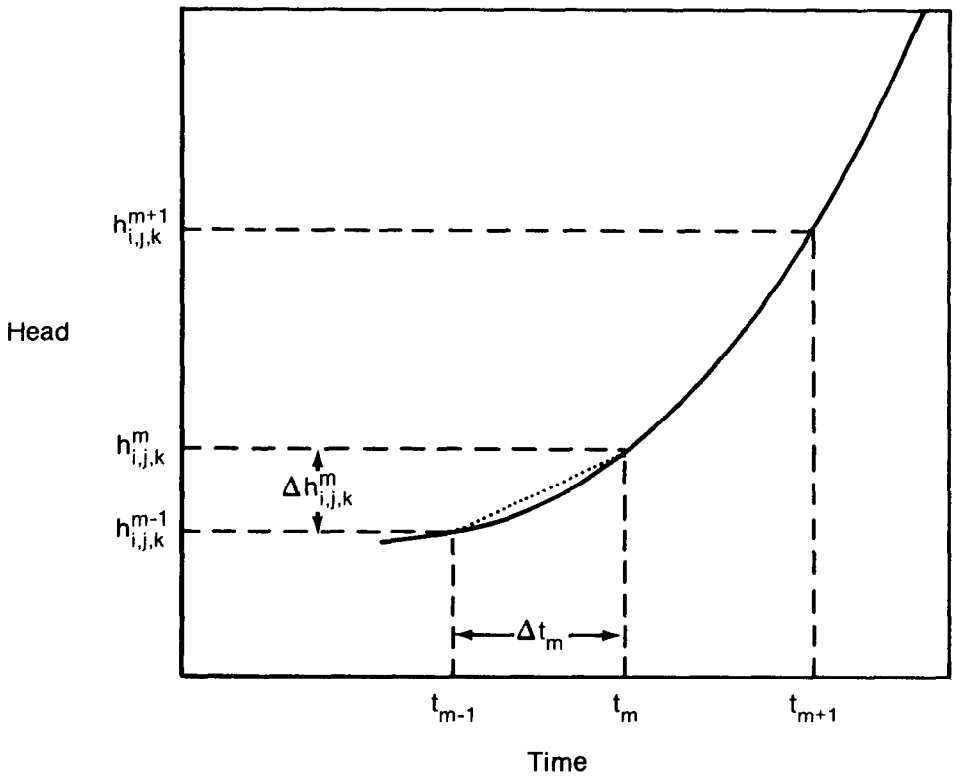
Equations (10) through (15) and (21) may be substituted into equation (22) to give the finite-difference approximation for cell i,j,k as

$$CR_{i,j-1/2,k}(h_{i,j-1,k} - h_{i,j,k}) + CR_{i,j+1/2,k}(h_{i,j+1,k} - h_{i,j,k})$$
$$+ CC_{i-1/2,j,k}(h_{i-1,j,k} - h_{i,j,k}) + CC_{i+1/2,j,k}(h_{i+1,j,k} - h_{i,j,k})$$
$$+ CV_{i,j,k-1/2}(h_{i,j,k-1} - h_{i,j,k}) + CV_{i,j,k+1/2}(h_{i,j,k+1} - h_{i,j,k})$$
$$+ P_{i,j,k}h_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}(\Delta r_j \Delta c_i \Delta v_k)\Delta h_{i,j,k}/\Delta t. \tag{23}$$

The finite-difference approximation for the time derivative of head, $\frac{\Delta h_{i,j,k}}{\Delta t}$ must next be expressed in terms of specific heads and times. Figure 6 shows a hydrograph of head values at node i,j,k. Two values of time are shown on the horizontal axis: t_m, which is the time at which the flow terms of equation (23) are evaluated; and t_{m-1}, a time which 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,

$$\left(\frac{\Delta h_{i,j,k}}{\Delta t}\right)_m \doteq \frac{h^{m}_{i,j,k} - h^{m-1}_{i,j,k}}{t_m - t_{m-1}}$$

Thus the hydrograph slope, or time derivative, is approximated using the change in head at the node over a time interval which 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 which extends backward in time from t_m, the time at which the flow terms are calculated. There are other ways in which $\Delta h/\Delta t$ could be approximated; for example, we could approximate it over a time interval which begins at the time of flow evaluation and extends to some later time; or over a time interval which 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.



Explanation

t_m	time at end of time step m
$h^m_{i,j,k}$	head at node i,j,k at time t_m
.....	Backward difference approximation to slope of hydrograph at time t_m

Figure 6.—Hydrograph for cell i,j,k.

In an unstable situation, errors which enter the calculation for any reason at a particular time will increase at each succeeding time as the calculation progresses, until finally they 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 it leads to large systems of equations which must be solved simultaneously for each time at which heads are to be computed.

Equation (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:

$$CR_{i,j-1/2,k}(h^m_{i,j-1,k} - h^m_{i,j,k}) + CR_{i,j+1/2,k}(h^m_{i,j+1,k} - h^m_{i,j,k})$$
$$+ CC_{i-1/2,j,k}(h^m_{i-1,j,k} - h^m_{i,j,k}) + CC_{i+1/2,j,k}(h^m_{i+1,j,k} - h^m_{i,j,k})$$
$$+ CV_{i,j,k-1/2}(h^m_{i,j,k-1} - h^m_{i,j,k}) + CV_{i,j,k+1/2}(h^m_{i,j,k+1} - h^m_{i,j,k})$$
$$+ P_{i,j,k}h^m_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}(\Delta r_j \Delta c_i \Delta v_k)\frac{(h^m_{i,j,k} - h^{m-1}_{i,j,k})}{t_m - t_{m-1}}. \quad (24)$$

Equation (24) is a backward-difference equation which can be used as the basis for a simulation of the partial differential equation of ground water flow, equation (1). Like the term $Q_{i,j,k}$, the coefficients of the various head terms in equation (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 (24) cannot be solved independently, since it represents a single equation in seven unknowns. However, an equation of this type can be written for each active cell in the mesh; and, since there is only one unknown head 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 $h^1_{i,j,k}$ at each point in the mesh---that is, it 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 $h^2_{i,j,k}$--that is, heads at time t_2, which marks the end of the first time step. In equation (25), therefore, the head superscript m is taken as 2, while the superscript m-1, which appears in only one head term, is taken as 1. The equation therefore becomes

$$CR_{i,j-1/2,k}(h^2_{i,j-1,k} - h^2_{i,j,k}) + CR_{i,j+1/2,k}(h^2_{i,j+1,k} - h^2_{i,j,k})$$

$$+ CC_{i-1/2,j,k}(h^2_{i-1,j,k} - h^2_{i,j,k}) + CC_{i+1/2,j,k}(h^2_{i+1,j,k} - h^2_{i,j,k})$$

$$+ CV_{i,j,k-1/2}(h^2_{i,j,k-1} - h^2_{i,j,k}) + CV_{i,j,k+1/2}(h^2_{i,j,k+1} - h^2_{i,j,k})$$

$$+ P_{i,j,k}h^2_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}\frac{(\Delta r_j \Delta c_i \Delta v_k)(h^2_{i,j,k} - h^1_{i,j,k})}{t_2 - t_1} \qquad (25)$$

where again the superscripts 1 and 2 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 mesh 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_2. When these have been obtained, the process is repeated to obtain heads at time t_3, the end of the second time step. To do this, equation (25) is reapplied, now using 2 as time subscript m-1 and 3 as time subscript m. Again, a system of equations is formulated, where the unknowns are now the heads at time t_3; and this set of equations is solved simultaneously to obtain the head distribution at time t_3. This process is continued for as many time steps as necessary to cover the time range of interest.

It is important to note that the set of finite-difference equations is reformulated at each time step; that is, at each 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.

Iteration

The model described in this report 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 which alters these estimated values, producing a new set of head values which 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 which more nearly satisfies the system of equations. Each repetition of the calculation is termed an "iteration." Ultimately, as the interim heads approach values which would exactly satisfy the set of equations, the changes produced by succeeding stages of calculation become very small. This behaviour 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 mesh. In figure 7, these arrays are represented as three-dimensional lattices, each identified by an array symbol, $\overline{h}$, bearing two superscripts. The first superscript indicates the time step for which the heads in the array are calculated, while the second indicates the number, or level, of the iteration which produced the head array. Thus $\overline{h}^{m,2}$ represents the array of values computed in the first iteration for the end of step m; $\overline{h}^{m,2}$ would represent the array of values computed in the second iteration; and so on. The head values which were initially assumed for the end of time step m, to begin the process of iteration, appear in the array designated $\overline{h}^{m,o}$. In the example of figure 7, 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 $\overline{h}^{m,n}$. Figure 7 also shows the array of final head values for the end of the preceding time step $\overline{h}^{m-1,n}$ (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 (24)--i.e., they are used in the term $h^{m-1}_{i,j,k}$ on the right side of equation (24)--in the calculation of heads for time step m. Because they represent heads for the preceding time step, for which computations have

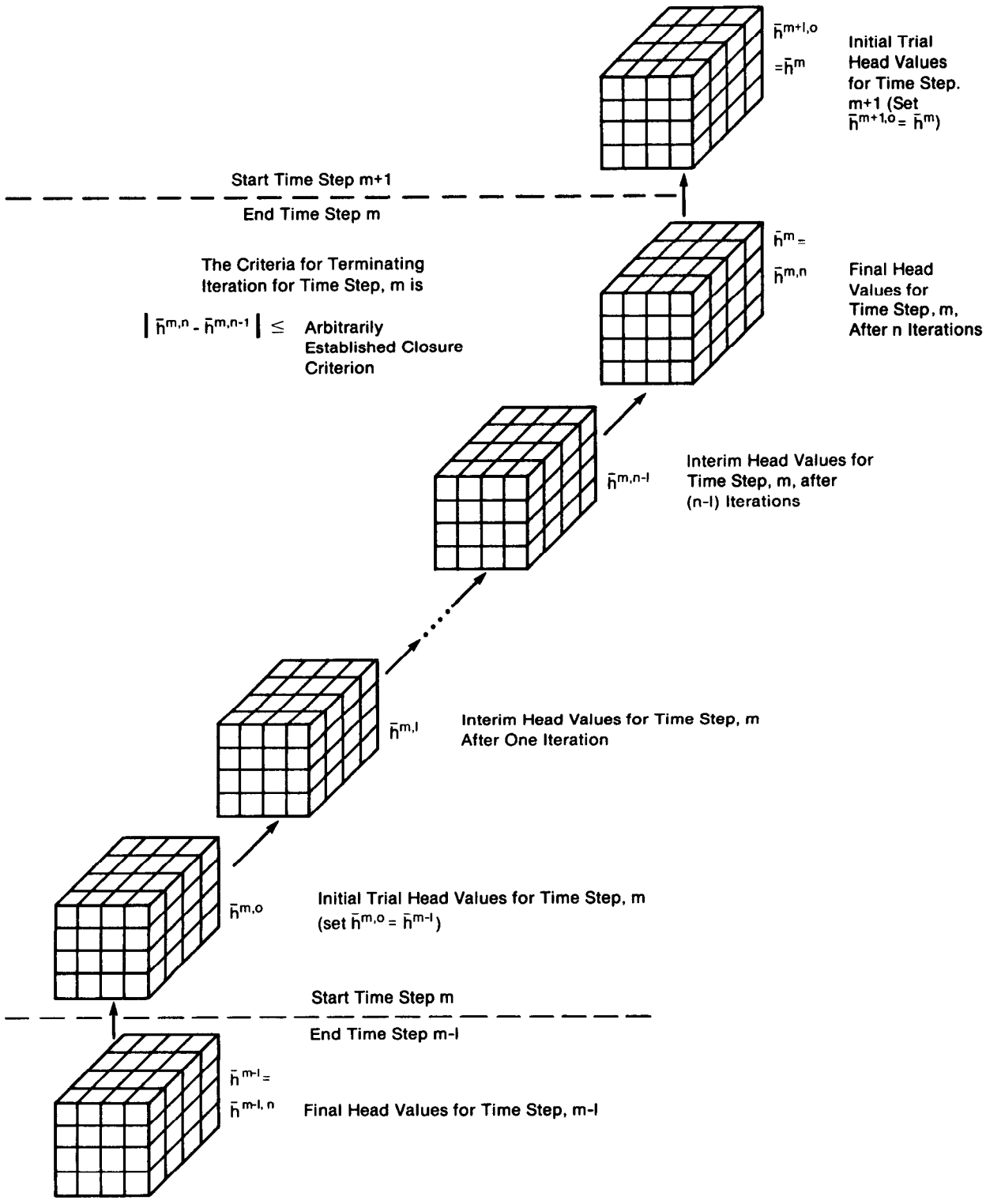


Figure 7.—Iterative calculation of a head distribution.

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.

Ideally, one would like to specify that iteration stop when the calculated heads are suitably close to the exact solution. However, because the actual solution is unknown, 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 occuring 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 mesh. 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 it 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.

The program described herein also incorporates a maximum permissible number of iterations per time step. If closure is not achieved within this maximum number of iterations, the iterative process will be terminated and a

corresponding message printed in the output. The closure criterion is designated HCLOSE in the model input, while the maximum number of iterations per time step is designated MXITER.

The initial estimates of head for the end of time step m, in array $\overline{h}^{m,o}$ of figure 7, 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 the model described in this report, the heads computed for the end of each time step are used as the initial trial values of head for the end of the succeeding time step. Thus in figure 7, the array $\overline{h}^{m-1,n}$ 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 $\overline{h}^{m,o}$, and used as the initial estimates, or trial values, for the heads at the end of time step m. Head values for the end of 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 may be found in many standard references, including Peaceman (1977), Crichlow (1977) and Remson, Hornberger and Molz (1971). It is suggested that the reader 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 Chapters 12 and 13 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 which is employed. However, it is important to note that even if exact solutions to the set of finite-difference equations were obtained at each step, these exact solutions would themselves be only an approximation to the solution of the differential equation of flow (equation (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 $h(x_i,y_j,z_k,t_m)$ 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 mesh spacing and time-step length are increased. Finally, it must be recognized that even if a formal solution of the differential equation could be obtained, it would normally 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.

Formulation of Equations for Solution

The model described in this report presently incorporates two 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 (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. The resulting equation is

$$CV_{i,j,k-1/2}h^{m}_{i,j,k-1} + CC_{i-1/2,j,k}h^{m}_{i-1,j,k} + CR_{i,j-1/2,k}h^{m}_{i,j-1,k}$$

$$+ (-CV_{i,j,k-1/2} - CC_{i-1/2,j,k} - CR_{i,j-1/2,k} - CR_{i,j+1/2,k}$$

$$- CC_{i+1/2,j,k} - CV_{i,j,k+1/2} + HCOF_{i,j,k})h^{m}_{i,j,k} + CR_{i,j+1/2,k}h^{m}_{i,j+1,k}$$

$$+ CC_{i+1/2,j,k}h^{m}_{i+1,j,k} + CV_{i,j,k+1/2}h^{m}_{i,j,k+1} = RHS_{i,j,k} \qquad (26)$$

where

$$HCOF_{i,j,k} = P_{i,j,k} - SC1_{i,j,k}/(t_m - t_{m-1}); \qquad (L^2t^{-1})$$

$$RHS_{i,j,k} = - Q_{i,j,k} - SC1_{i,j,k}h^{m-1}_{i,j,k}/(t_m - t_{m-1}); \text{ and} \qquad (L^3t^{-1})$$

$$SC1_{i,j,k} = SS_{i,j,k}\Delta r_j \Delta c_i \Delta v_k. \qquad (L^2)$$

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

$$[A]\{h\} = \{q\} \qquad (27)$$

where [A] is a matrix of the coefficients of head, from the left side of equation (26), for all active nodes in the mesh; {h} is a vector of head values at the end of time step m for all nodes in the mesh; and {q} is a vector of the constant terms, RHS, for all nodes of the mesh. The model described in this report assembles the vector {q} and the terms that comprise [A] through a series of subroutines, or "modules". The vector {q} and the terms comprising [A] are then transferred to modules which actually solve the matrix equations for the vector {h} .

Types of Model Cell and Simulation of Boundaries

In practice, it is generally unnecessary to formulate an equation of the form of (24) for every cell in a model mesh, as the status of certain cells is specified in advance in order to simulate the boundary conditions of the problem. In the model described in this report, cells of this type are grouped into two categories--"constant-head" cells and "inactive" (or "no-flow") cells. Constant-head cells are those for which the head is specified in advance, and is held at this specified value through all time steps of the simulation. Inactive or no-flow cells are those for which no flow into or out of the cell is permitted, in any time step of the simulation. The remaining cells of the mesh, termed "variable-head" cells in this report, are characterized by heads which are unspecified and free to vary with time. An equation of the form of (24) must be formulated for each variable-head cell in the mesh, 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 the model described herein to represent conditions along various hydrologic boundaries. For example, figure 8 shows the map of an aquifer boundary superimposed on an array of cells generated for the model. The aquifer is of irregular shape, whereas the model array is always rectangular in outline; no-flow cells have therefore been used to delete the portion of the array 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 or through a combination of no-flow cells and external source terms.

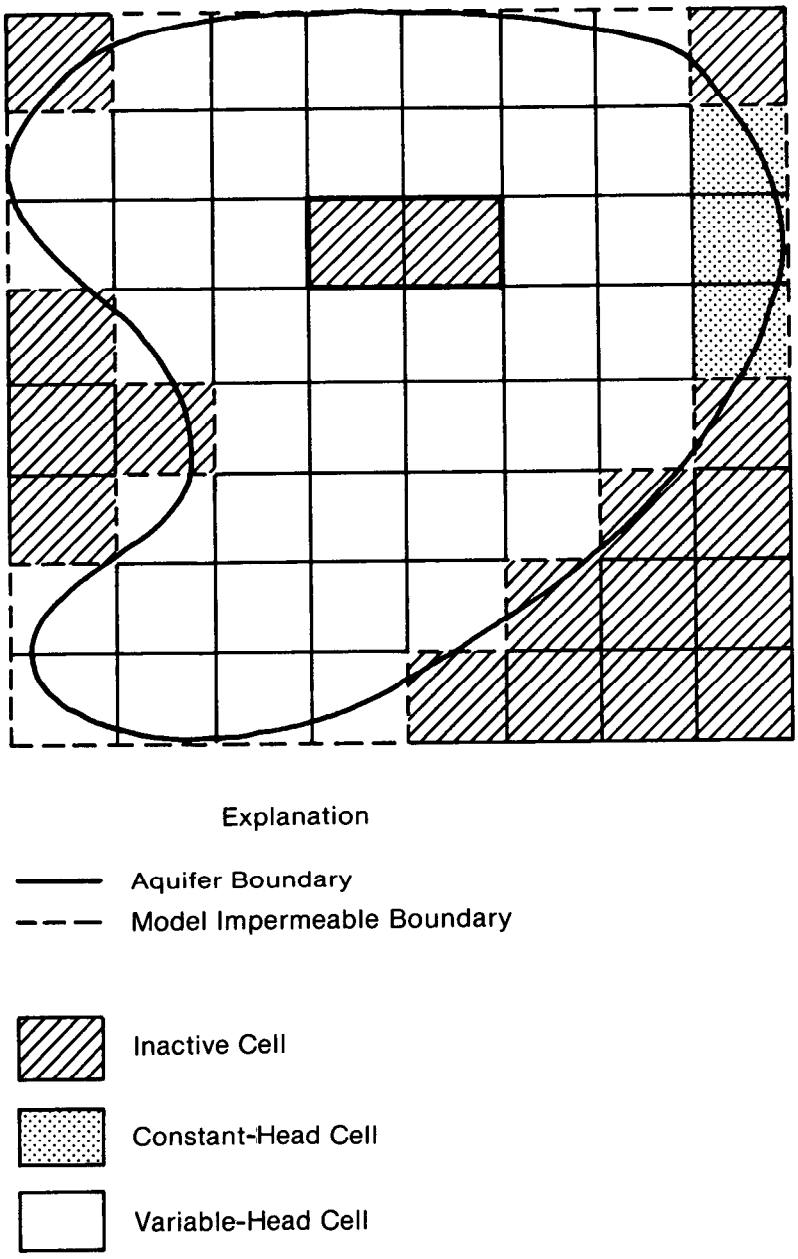
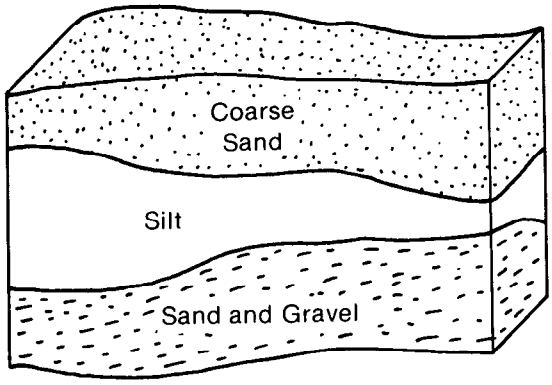


Figure 8.—Discretized aquifer showing boundaries and cell designations.

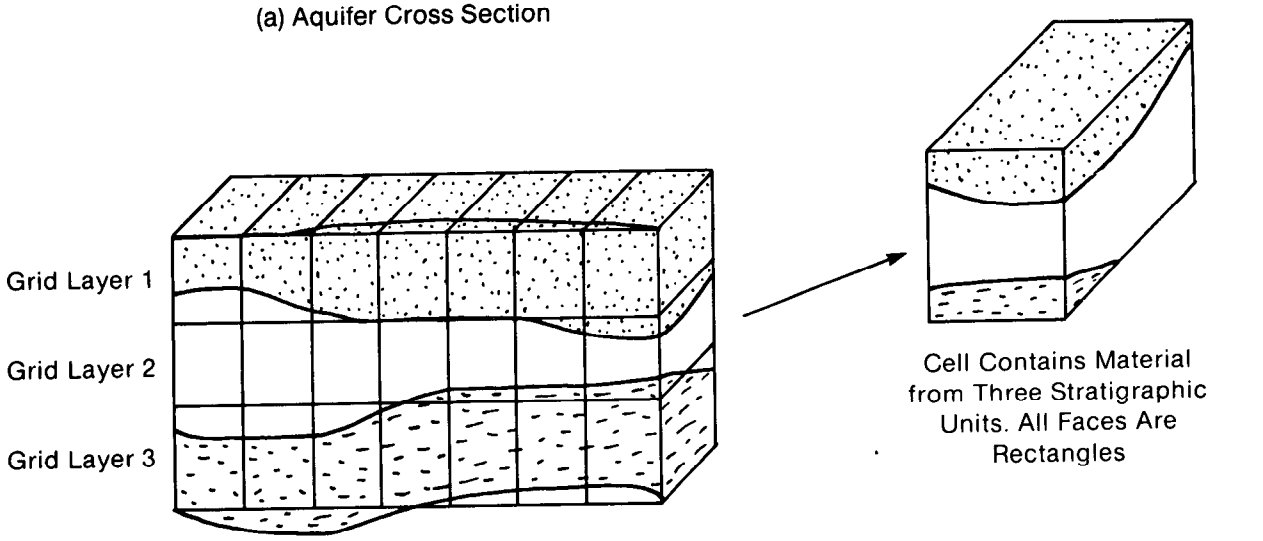
Conceptual Aspects of Vertical Discretization

The model described in this document 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 hydraulic parameters which contain or embody the layer thickness. This approach is followed in preference to explicit reading of layer thickness in order to accomodate two different ways of viewing vertical discretization.

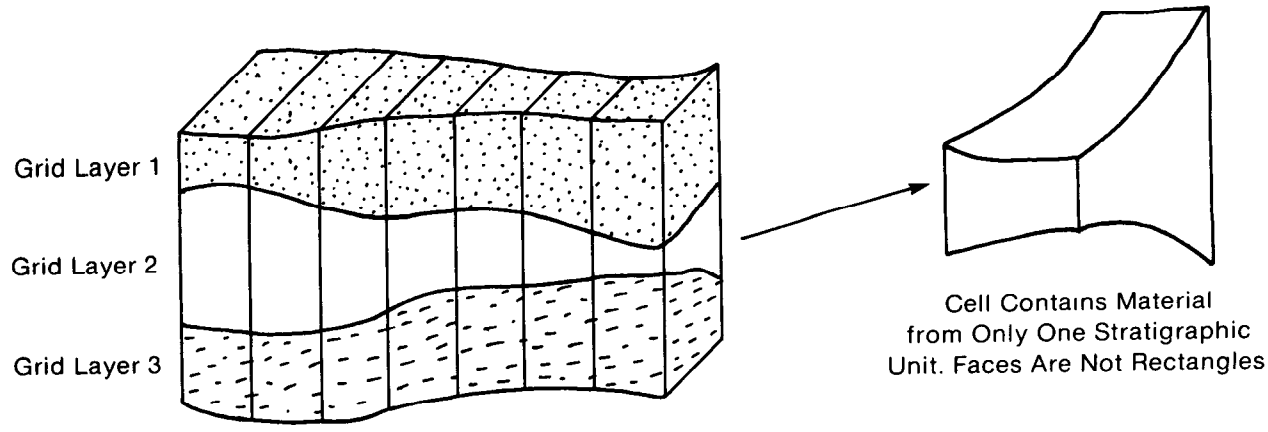
At one extreme, vertical discretization can be visualized simply as an extension of areal discretization--a more or less arbitrary process of dividing the flow system into segments along the vertical, governed in part by the vertical resolution desired in the results. At the opposite extreme, vertical discretization can be viewed as an effort to represent individual aquifers or permeable zones by individual layers of the model. Figure 9-a shows a typical geohydrologic sequence which has been discretized according to both interpretations--in 9-b according to the first viewpoint, and in 9-c according to the second. The first viewpoint leads to rigid superposition of an orthogonal three-dimensional mesh on the geohydrologic system; while there may be a general correspondence between geohydrologic layers and model layers, no attempt is made to make the mesh conform to stratigraphic irregulaties. Under the second viewpoint, model layer thickness is considered variable, to simulate the varying thickness of geohydrologic units; this leads, in effect, to a deformed mesh.



(a) Aquifer Cross Section



(b) Aquifer Cross Section With
Rectilinear Grid Superimposed



(c) Aquifer Cross Section With
Deformed Grid Superimposed

Figure 9.—Schemes of vertical discretization.

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 parameters can be specified for each cell; these conditions are more likely to be met when model layers conform to geohydrologic units as in figure 9-c. 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 9-c. On the other hand, the deformed mesh of 9-c fails to conform to many of the assumptions upon which the model equations are based; for example, individual cells may no longer have rectangular faces, and the major axes of hydraulic conductivity may not be aligned with the model axis. 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 9-b and 9-c. For example, even where layer boundaries conform to geohydrologic contacts, it may be necessary to use more than one layer to simulate a single geohydrologic unit, simply to achieve the resolution required in the results. Figure 10 shows a system consisting of two sand units separated by a clay; the units are of uniform thickness, and each could be represented by a single layer without deformation of the mesh. However, flow is neither fully horizontal nor fully vertical in any of the layers; if information on the direction of flow within each unit is required, several layers must be used to represent each unit. Similarly, figure 11 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

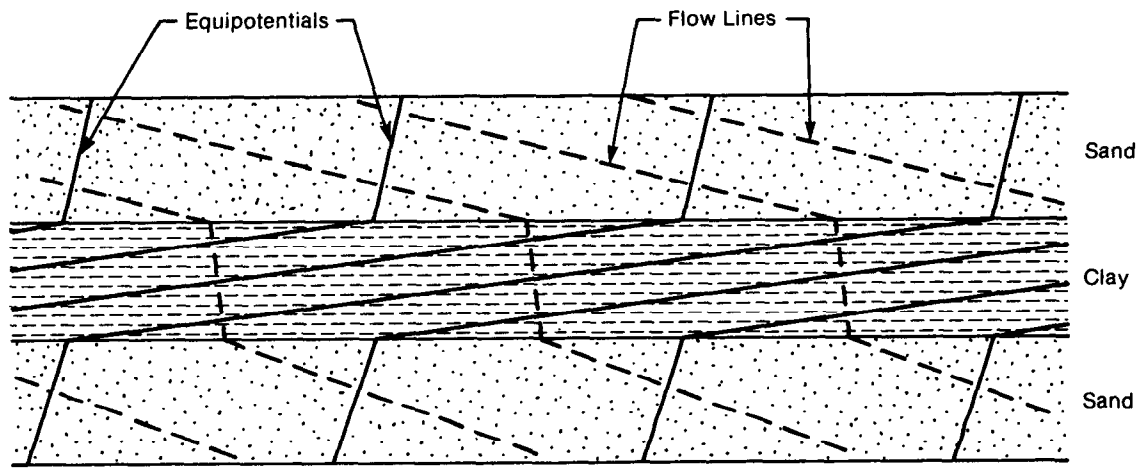


Figure 10.—Possible pattern of flow in a cross section consisting of two high conductivity units separated by a low conductivity unit.

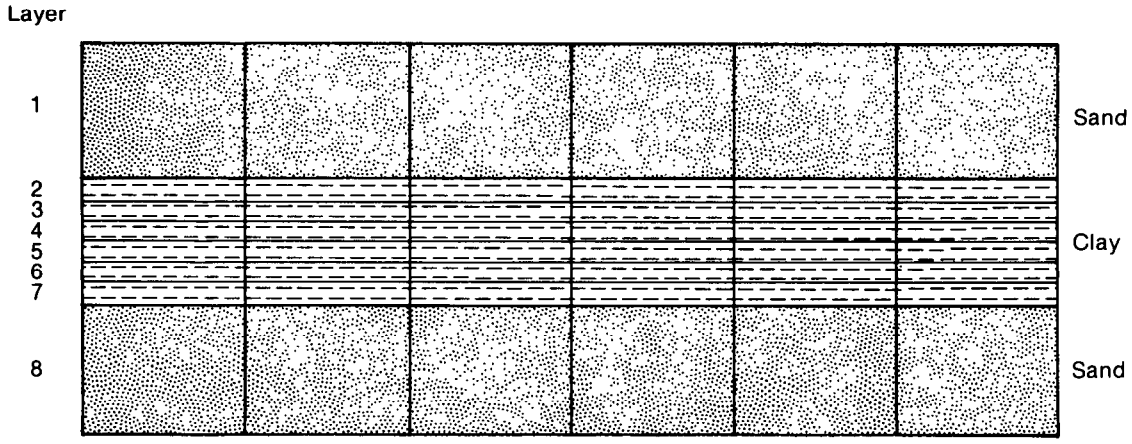


Figure 11.—A cross section in which a low conductivity unit is represented by six model layers.

required to represent that unit, as shown in the figure. On the other hand, figure 12 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, while the clay may be represented simply by the vertical conductance between layers. This approach to vertical discretization has sometimes been termed the "quasi three-dimensional" approach.

The approaches to vertical discretization described above all lead to a set of equations of the form of (26), which must be solved simutaneously 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. The model described in this document is capable of implementing any of these approaches to vertical discretization in that, as noted above, the thickness of individual layers (Δv_k of figure 1 and equation (24)) is never read explicitly by the program; rather, this thickness is embedded in various hydraulic coefficients specified by the user. For example, in confined layers transmissivity, which is the product of hydraulic conductivity and layer thickness, is specified; and storage coefficient, the product of specific storage and layer thickness, is also used. For an unconfined layer, aquifer bottom elevation and hydraulic conductivity are input for each cell. Saturated thickness is calculated as head minus bottom elevation, and transmissivity is then calculated as hydraulic conductivity times saturated thickness. Thus, layer thickness can vary from cell to cell depending on bottom elevation and head. Chapter 5, which describes the Block Centered Flow Package, contains a discussion of the formulation of conductance and storage terms corresponding to the various ways of conceptualizing the vertical discretization.

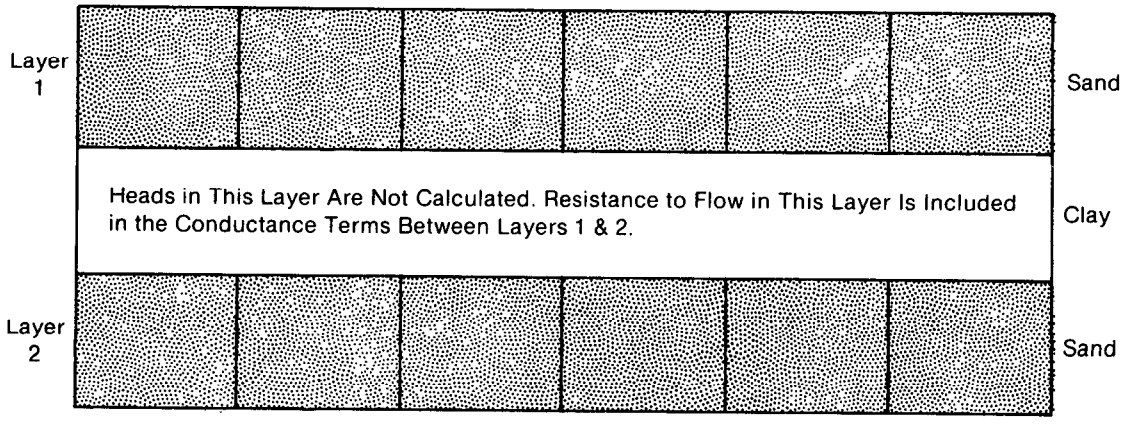


Figure 12.—A cross section in which a low conductivity unit is represented by the conductance between model layers.