THREE DIMENSIONAL GROUNDWATER FLOW MODEL

MODEL DESCRIPTION

Mathematical Model

The governing partial differential flow equation for the three dimensional unsteady (transient) movement of incompressible groundwater through heterogeneous and anisotropic medium may be described as

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) - W = S_s\frac{\partial h}{\partial t} \quad ...(1)$$

where,

x,y,z are the cartesion coordinates aligned along the major axes of conductivity K_{xx}, K_{yy}, K_{zz};

h is the piezometric head (L);

W is the volumetric flux per unit volume and represents source and/or sinks (t^{-1});

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

t is time (t)

here,
$S_s = S_s(x,y,z)$
$K_{xx} = K_{xx}(x,y,z)$
$K_{yy} = K_{yy}(x,y,z)$

Lectured delivered by Mr. S.K. Singh, Scientist 'C'

$$K_{zz} = K_{zz}(x,y,z)$$
$$h = h(x,y,z,t)$$
$$W = W(x,y,z,t) \quad \ldots(2)$$

Thus, in general the specific storage and the conductivities may be the functions of space and time. Therefore, the flow under non-equilibrium conditions in a heterogeneous and anisotropic medium is described by equation 1. This equation when combined with boundary conditions (flow and/or head conditions at the boundaries of the aquifer system) and initial conditions (in case of transient flow, specification of head conditions at t=0), constitute a mathematical model of transient groundwater flow.

The analytical solutions of equation 1 is not feasible for complex systems, so various numerical methods must be employed to obtain approximate solutions. Finite difference approach is one of such numerical methods, wherein the continuous system described by equation 1 is replaced by a set of discrete points in space and time, and the partial derivatives are replaced by finite differences between functional values at these points. Thus, the process leads to systems of simultaneous linear algebraic difference equations,the solution of which yields values of head at specific points and time. These values are an approximation to the time varying head distribution that would be given by an analytical solution of the partial-differential equation of flow.

Discretization convention

For the formulation of finite difference equations, the aquifer system need to be discretized into a mesh of points termed nodes, forming rows, columns, and layers. Such spatial discretization of an aquifer system is shown in fig. 1. To conform with computer array convention, an i,j,k coordinate system is used. If an aquifer system consists 'nrow' rows, 'ncol' columns and 'nlay' layers, then

i is the row index, $i = 1,2,\ldots$ nrow;

j is the column index, $j = 1,2,\ldots$ ncol;

k is the layer index, $k = 1,2,\ldots$ nlay.

For example, fig. 1 shows a system with nrow=5 ncol=9 and nlay=5. With respect to cartesian coordinate system, points along a row are parallel to x axis, points along a column are parallel to the y axis, and points along vertical are parallel to z axis. In spatial discretization, nodes represent prisms of porous material termed cells in conceptual sense. Within each cell the hydraulic properties are constant so that any value associated with a node applies to or is distributed over the extent of a cell.

The width of cells along rows is designated as Δr_j for the j^{th} column; the width of cells along columns are designated as ΔC_i for i^{th} row; and the thickness of layers in vertical are designated as ΔV_k for the K^{th} layer (Fig. 1). Thus the cell with the coordinates of $(i,j,k) = (5,3,2)$ has a volume of $\Delta r_3 . \Delta C_5 . \Delta V_2$.

Configuration of cells

There exists two conventions for defining the configuration of cells with respect to the location of nodes, viz., the block centered formulation and the point centered formulation. In both systems the aquifer is divided with two sets of parallel lines which are perpendicular to each other.

In block-centered formulation, the blocks formed by the sets of parallel lines are the cells and the nodes are at the centre of the cells.

In point-centered formulation the nodes are assumed at the intersection points of the sets of parallel lines and the cells are drawn around the nodes with faces half way between nodes.

In either case of configuration, the spacing of nodes should be such that the hydraulic properties of the system are uniform over the extent of a cell. Both types of grid configurations have been shown in fig. 2.

Finite Difference Equation

The following development of finite difference equation holds good for both type of grid configuration described earlier. The groundwater flow equation may be written in finite difference form applying continuity equation. Thus, the sum of all flows into and out of cell must be equal to the rate of change of storage within the cell. Under the assumption that the groundwater is incompressible, the continuity equation (expressing the balance of flow) for a cell can be written as

$$\Sigma Q_i = S_s \frac{\Delta h}{\Delta t} . \Delta V \qquad \ldots(3)$$

where

Q_i is the flow rate into the cell ($L^3 t^{-1}$)

S_s is the specific storage defined as the ratio of 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);

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

Here, the right hand side of equation 3 represents the volume of water taken into the storage over a time interval Δt given a change in head of Δh. Thus, equation 3 is stated in terms of inflow and storage gain. Outflow and loss in storage are represented by defining outflow as negative inflow and loss as negative gain.

For a three dimensional problem each cell is surrounded by six adjacent cells. Fig. 3 shows a cell i,j,k and six adjacent cells, i.e., 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. Thus net flow to the cell i,j,k is the algebraic summation of the flows into the cell from six adjacent cells. Using Darcy's law, flow from each adjacent cell into the cell i,j,k can be obtained. Hence, flow into the cell i,j,k in row direction from cell i,j-1,k (fig. 4) is given by

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

where,

$q_{i,j-1/2,k}$ is the volumetric flow discharge through the face between the 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; and

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

The index j-1/2 indicates the space between nodes (fig. 4). It does not indicate a point exactly half way between nodes. For example, $KR_{i,j-1/2,k}$ represents hydraulic conductivity in the entire region between nodes i,j,k and i,j-1,k.

Since the grid dimensions and hydraulic conductivity remain constant throughout the solution process, the above equation may be rewritten by combining the constants into single constant called hydraulic conductance or simple 'conductance' of the cell.

$$q_{i,j-1/2,k} = CR_{i,j-1/2,k}(h_{i,j-1,k} - h_{i,j,k}) \qquad \ldots(5)$$

where $CR_{i,j-1/2,k} = KR_{i,j-1/2,k} \Delta c_i \Delta v_k / \Delta r_{j-1/2}$

$CR_{i,j-1/2,k}$ is the conductance in i^{th} row and k^{th} layer 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 devided by length of flow path; in this case, the distance between the nodes. Here, C represents the conductance and R represents in row direction.

Similar expressions can be written approximating the flows into or out of the cell i,j,k through the remaining five faces. Such expressions are as written below.

$$q_{i,j+1/2,k} = CR_{i,j+1/2,k}(h_{i,j+1,k} - h_{i,j,k}) \quad ...(6)$$

$$q_{i-1/2,j,k} = CC_{i-1/2,j,k}(h_{i-1,j,k} - h_{i,j,k}) \quad ...(7)$$

$$q_{i+1/2,j,k} = CC_{i+1/2,j,k}(h_{i+1,j,k} - h_{i,j,k}) \quad ...(8)$$

$$q_{i,j,k-1/2} = CV_{i,j,k-1/2}(h_{i,j,k-1} - h_{i,j,k}) \quad ...(9)$$

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

Equations 5 -10 represent the flow into the cell i,j,k from six adjacent cells. Seepage from the stream beds. drains,areal recharge, evapotranspiration and flow from wells are taken care of by additional terms which accounts for flow into the cell from outside the aquifer. These flows may depend on the head in the receiving cell but are independent of the heads in all other cells of the aquifer or they may be entirely independent of head in receiving cell. Flow from outside the aquifer which is represented by W in equation 1, may be represented in general as

$$a_{i,j,k,n} = p_{i,j,k}\, h_{i,j,k} + q_{i,j,k,n} \qquad \ldots(11)$$

where,

$a_{i,j,k,n}$ is the flow from the n-th external source into cell i,j,k $[L^3T^{-1}]$

$p_{i,j,k,n}$ is a constant $[L^2T^{-1}]$

$q_{i,j,k,n}$ is a constant $[L^3T^{-1}]$

For example, let cell i,j,k represents a well and $q_{i,j,k}$ represents discharge. $q_{i,j,k,1}$ is the discharge being pumped. In this case, the discharge from the well is assumed to be independent of head. Hence,

$p_{i,j,k,1}$ is zero and

$$a_{i,j,k,1} = -q_{i,j,k,1} \qquad \ldots(12)$$

If the second external source (n=2) is taken to be seepage from river bed, it is proportional to the head difference river stage ($R_{i,j,k}$) and head in the receiving cell i,j,k ($h_{i,j,k}$). Hence,

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

$$\text{or } a_{i,j,k,2} = -CRIV_{i,j,k,2}\, h_{i,j,k} + CRIV_{i,j,k,2}\, R_{i,j,k} \qquad \ldots(13)$$

where $CRIV_{i,j,k,2}$ is the conductance of the river bed in cell i,j,k $[L^2T^{-1}]$

The conductance $CRIV_{i,j,k,2}$ corresponds to $p_{i,j,k,2}$ and 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 11. If there are N external sources or stresses affecting a single cell, the combined flow is expressed by

$$QS_{i,j,k} = \sum_{n=1}^{N} a_{i,j,k,n}$$

$$= \sum_{n=1}^{N} p_{i,j,k,n}\, h_{i,j,k} + \sum_{n=1}^{N} q_{i,j,k,n}$$

$$= P_{i,j,k}\, h_{i,j,k} + Q_{i,j,k}$$

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

and $Q_{i,j,k} = \sum_{n=1}^{N} q_{i,j,k,n}$ ...(14)

While writing the continuity equation of the form given by equation 3, for cell i,j,k, the term ΣQ_i consists of flow to the cell from six adjacent cells, and all other external flow rate to the cell. The flow from six adjacent cells into cell i,j,k is given by equations 5- 10 and the flow from the external sources into cell i,j,k is represented by equation 14. Substituting these equations in equation 3, we get

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

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

$$CC_{i-1/2,j,k}(h_{i-1,j,k} - h_{i,j,k}) +$$

$$CC_{i+1/2,j,k}(h_{i+1,j,k} - h_{i,j,k}) +$$

$$CV_{i,j,k-1/2}(h_{i,j,k-1} - h_{i,j,k}) +$$

$$CV_{i,j,k+1/2}(h_{i,j,k+1} - h_{i,j,k}) +$$

$$P_{i,j,k}\, h_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}\,(\Delta r_j \Delta C_i \Delta V_k).(\Delta h_{i,j,k}/\Delta t)$$

...(15)

where, $\Delta h_{i,j,k}/\Delta t$ is a finite difference approximation for head change with respect to time $[LT^{-1}]$

$SS_{i,j,k}$ is 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 $[L^3]$

The above equation can be written in backward difference form by specifying flow term 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, i.e.,

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

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

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

$$+P_{i,j,k}h^m_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}(\Delta r_j \Delta C_i \Delta V_k)\frac{(h^m_{i,j,k} - h^{m-1}_{i,j,k})}{t_m - t_{m-1}}$$

...(16)

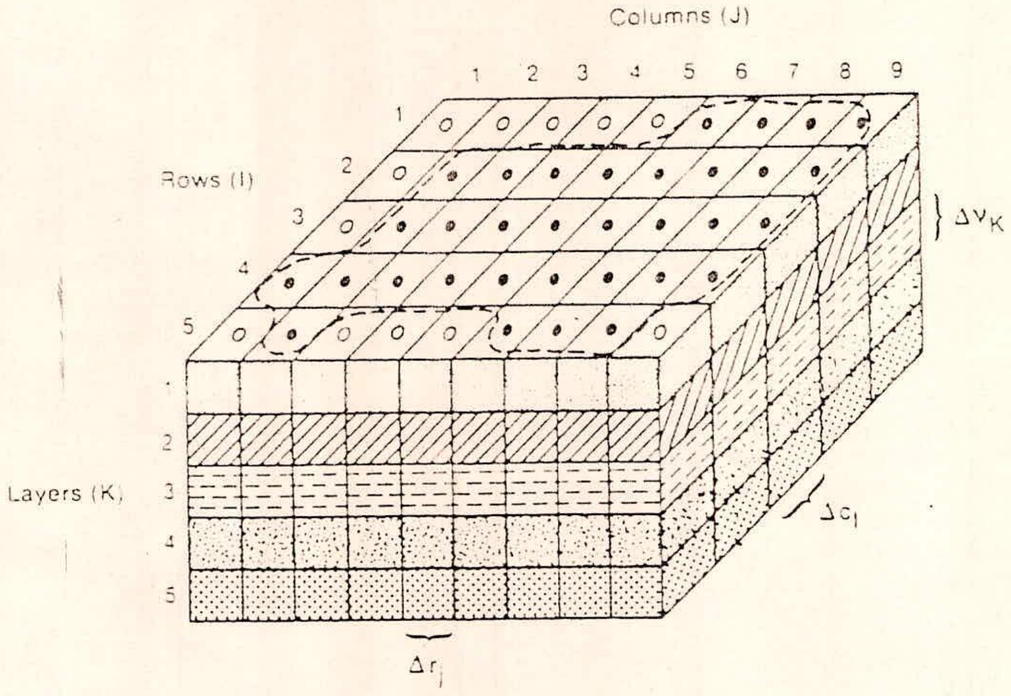
An equation of the above type for each of the 'n' cells in the system; and, since there is only one unknown head for each cell, we are left with a system 'n' equations and 'n' unknowns. Such a system of equations can be solved simultaneously.

Provision for Boundary Conditions and Initial Condition

The type of boundaries that may be imposed in the model include constant head, no-flow, constant flow, and head dependent flow. These various types of boundaries are represented by the difference cell types. Cells can be designated by three types viz, inactive cell; constant head cell; and, variable head cell. Variable head cells are those in which head vary with time. Therefore, an equation of the type of equation 16 is required for each variable head cell. Head remains constant with time in constant head cells and these cells do not require an equation, however, the adjacent variable head cells will contain non-zero conductance terms representing flow from the constant head cell. 'No flow cells' are those to which there is no flow from adjacent cells. Neither an equation is formulated for a no flow cell nor the equations for the adjacent cells contain a term representing flow from the no flow cell. The use of no-flow and constant head cells to simulate boundary conditions is given in fig. 5.Constant-flow and head-dependent flow boundaries can be represented by a combination of no-flow cells and external sources.

Solution

In most cases, the actual number of equations of the form of equation 16 will be less than the total number of model cells. This is because the number of equations is only equal to the number of 'variable head cells'. The objective of transient simulation is to predict the head distribution at successive times with the given initial head distribution and the boundary conditions. The initial head distribution consists of a value of $h^1_{i,j,k}$ at each point in the mesh at time t_1, 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 $h^2_{i,j,k}$, i.e., head at time t_2 which mark the end of the first time step. Therefore, in equation 16, the subscript m is taken as 2 and thus the subscript m-1, which appear in only one head term, is taken as 1. Once such equations are formed for each variable head cells, an iterative method is used to obtain the values of $h^2_{i,j,k}$. An iterative method starts with an initial trial solution. This trial solution is used to calculate through a procedure of calculation, an interim solution which more nearly satisfies the system of equations. The interim solution then becomes a new trial solution and the procedure is repeated. Each repetition is called an 'iteration'. The process is repeated until an iteration occurs in which the trial solution and the interim solution are nearly equal, i.e., for each node, the difference between the trial head value and the interim head value is smaller than some arbitrary established value, usually termed as 'closure criterion'. The interim solution is then regarded as a good approximation to the solution of system of equation under given initial and boundary conditions.



Explanation

- - - - Aquifer Boundary

● Active Cell

0 Inactive Cell

Δr_J Dimension of Cell Along the Row Direction. Subscript (J) Indicates the Number of the Column

Δc_I Dimension of Cell Along the Column Direction. Subscript (I) Indicates the Number of the Row

Δv_K Dimension of the Cell Along the Vertical Direction. Subscript (K) Indicates the Number of the Layer

Figure 1.—A discretized hypothetical aquifer system.

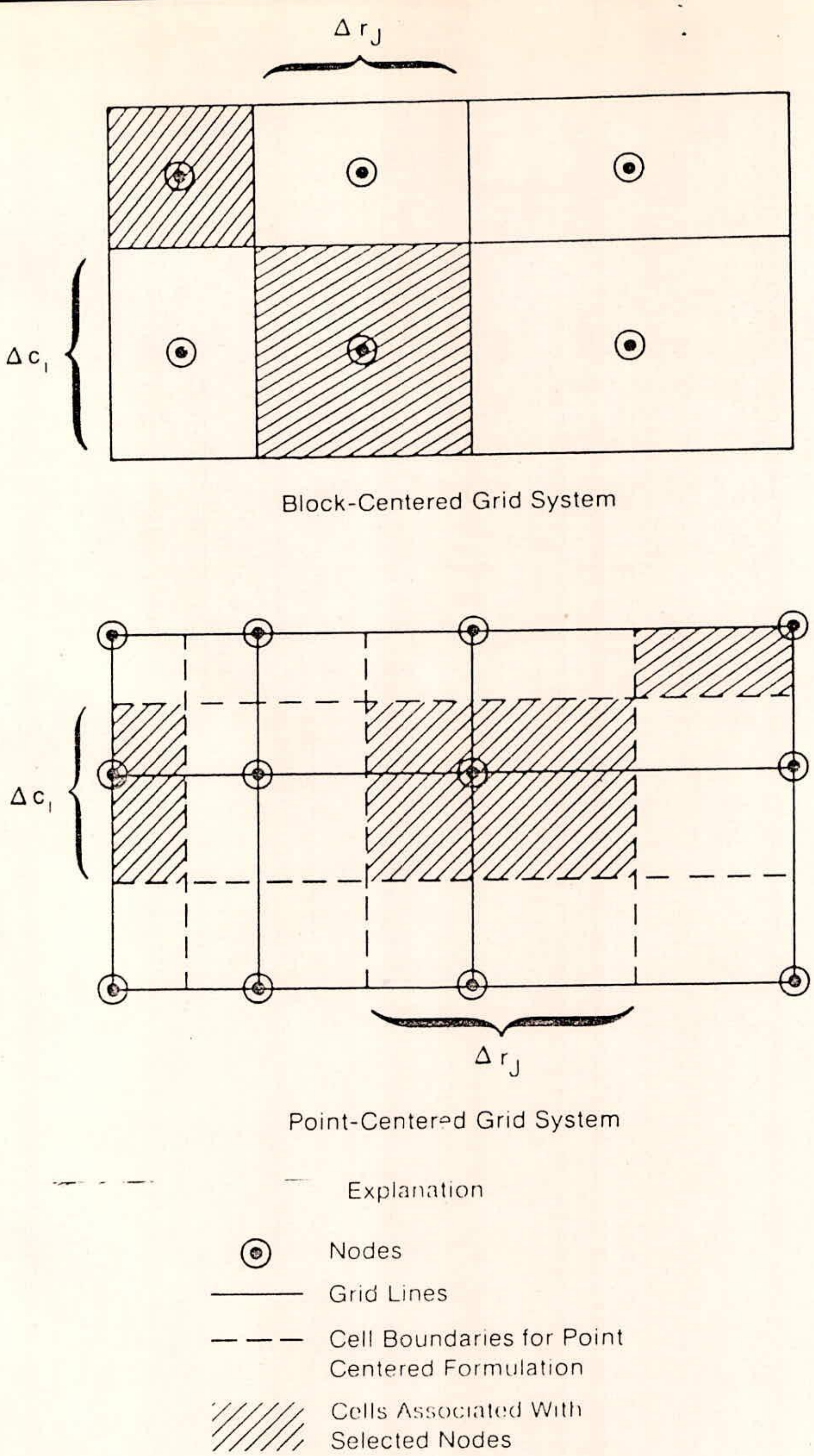


Figure 2.—Grids showing the difference between block-centered and point-centered grids.

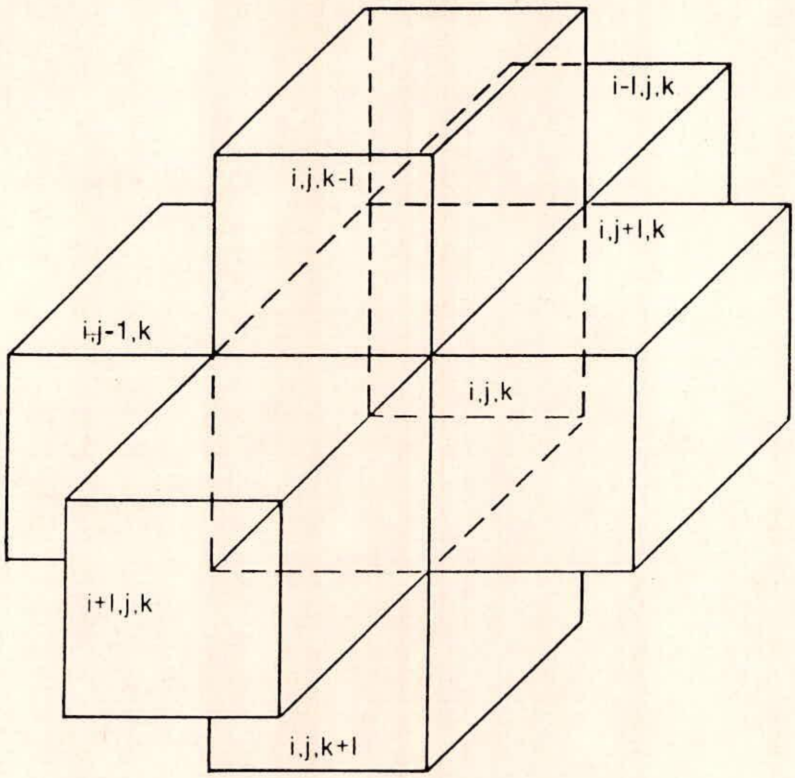


Figure 3.—Cell i,j,k and indices for the six adjacent cells.

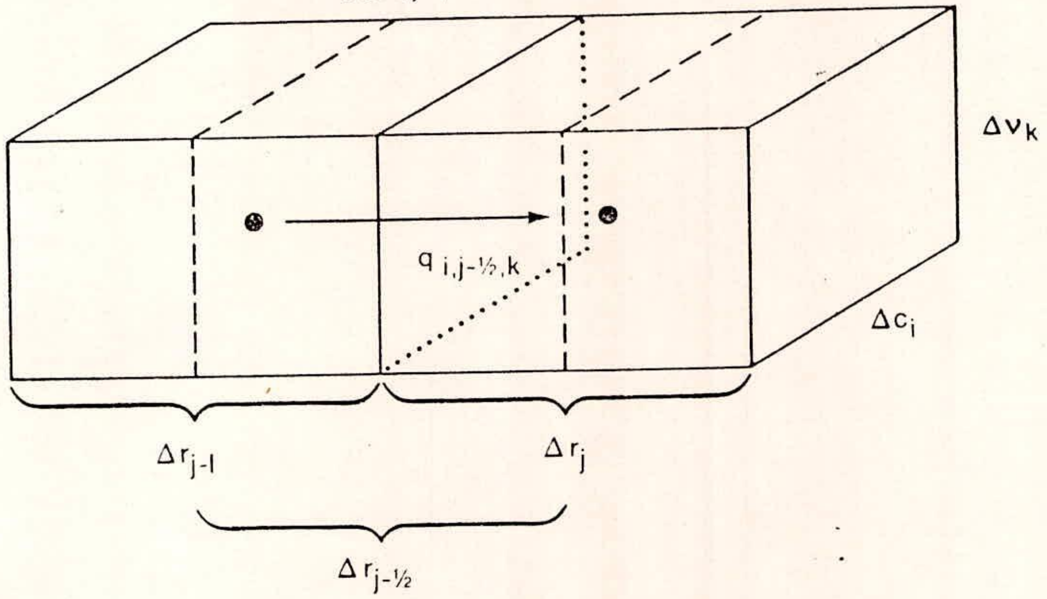


Figure 4.—Flow into cell i,j,k from cell i,j-l,k.

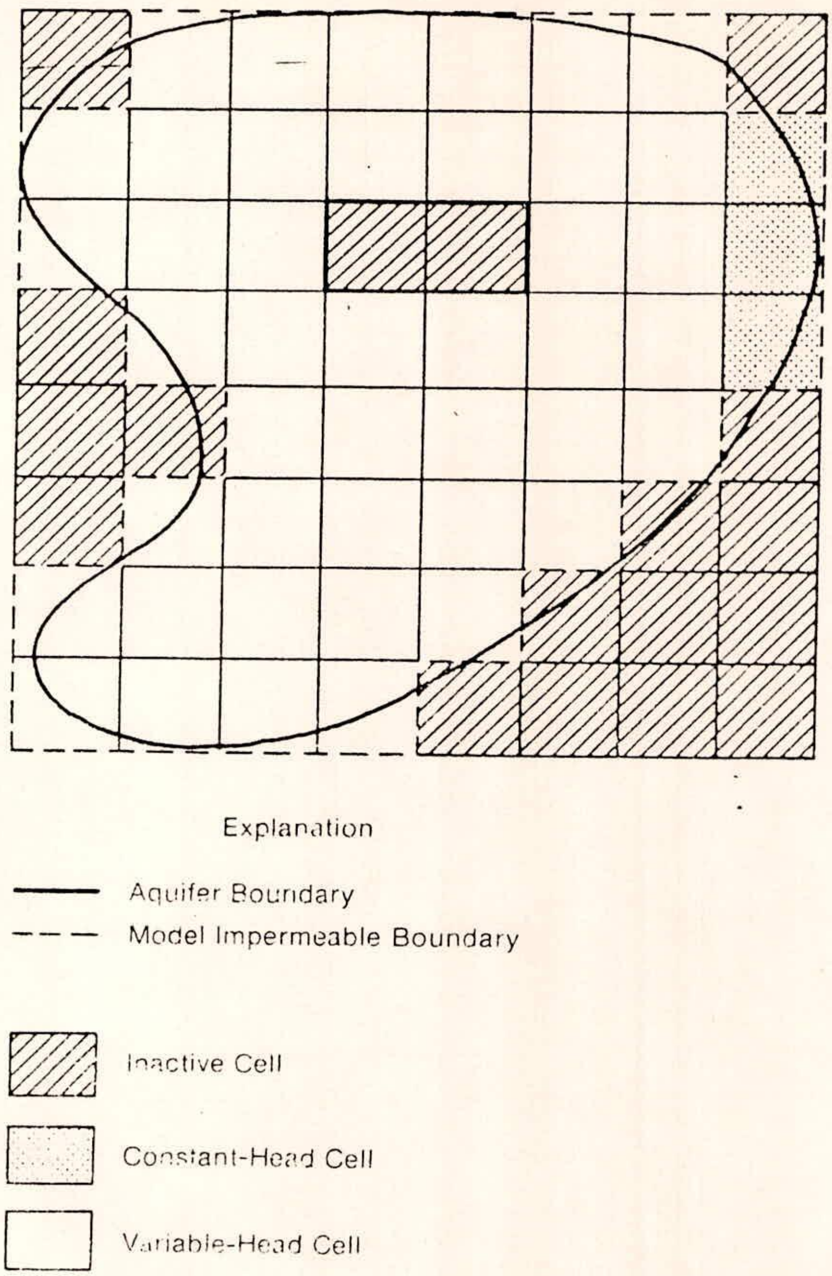


Fig. 5 - Discretized aquifer showing boundaries and constant head cells.