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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

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CHAPTER 5

BLOCK-CENTERED FLOW PACKAGE

Conceptualization and Implementation

The Block-Centered Flow (BCF) Package computes the conductance components of the finite-difference equation which determine flow between adjacent cells. It also computes the terms that determine the rate of movement of water to and from storage. To make the required calculations, it is assumed that a node is located at the center of each model cell; thus the name Block-Centered Flow is given to the package.

In Chapter 2, the equation of flow for each cell in the model was developed as

$$\begin{aligned} & CV_{i,j,k-1/2}h_{i,j,k-1}+CC_{i-1/2,j,k}h_{i-1,j,k}+CR_{i,j-1/2,k}h_{i,j-1,k} \\ & + (-CV_{i,j,k-1/2}-CC_{i-1/2,j,k}-CR_{i,j-1/2,k}-CR_{i,j+1/2,k} \\ & - CC_{i+1/2,j,k}-CV_{i,j,k+1/2}+HCOF_{i,j,k})h_{i,j,k}+CR_{i,j+1/2,k}h_{i,j+1,k} \\ & + CC_{i+1/2,j,k}h_{i+1,j,k}+CV_{i,j,k+1/2}h_{i,j,k+1} = RHS_{i,j,k}. \qquad (29) \end{aligned}$$

The CV, CR, and CC coefficients are conductances between nodes--sometimes called "branch conductances." The HCOF and RHS coefficients are composed of external source terms and storage terms. Besides calculating the conductances and storage terms, the BCF Package calculates flow-correction terms that are added to HCOF and RHS when an underlying aquifer becomes partially unsaturated. Under these conditions the flow to the underlying aquifer no longer increases in proportion to the head difference between aquifers, but rather reaches a constant limiting value. The additional terms correct the flow equations, in effect reducing the expressions for downward flow to correspond to this limiting value.

The following discussion of the conceptualization and implementation of the BCF package is divided into nine sections: Basic Conductance Equations, Horizontal Conductance Under Confined Conditions, Horizontal Conductance Under Water Table Conditions, Vertical Conductance Formulation, Vertical Flow Calculation Under Desaturating Conditions, Storage Formulation, Storage Term Conversion, Applicability and Limitations of Optional Formulations and Data Requirements.

Basic Conductance Equations

The concept of hydraulic conductance was introduced in Chapter 2 (equation (9)). It is reviewed here and extended to cover the calculation of equivalent conductance for elements arranged in series.

Conductance is a combination of several parameters used in Darcy's law. Darcy's law defines one-dimensional flow in a prism of porous material (figure 23) as

$$Q = KA(h_2-h_1)/L \qquad (30)$$

where

Q is the flow (L^3t^{-1});

K is the hydraulic conductivity of the material in the direction of flow (Lt^{-1});

A is the cross-sectional area perpendicular to the flow (L^2);

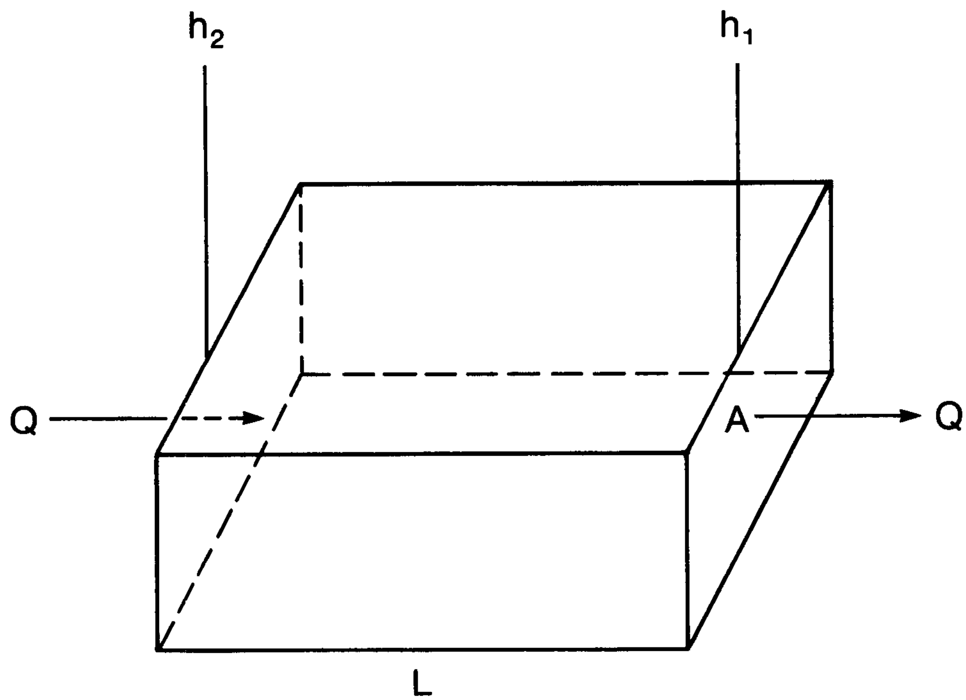
h_2-h_1 is the head differences across the prism parallel to flow (L); and

L is the length of the flow path (L).

Conductance, C, is defined as

$$C = KA/L. \qquad (31)$$

$$Q = \frac{KA\,(h_2 - h_1)}{L}$$



Explanation

K	Is Hydraulic Conductivity
h_2	Is the Head at the Left End of the Prism
h_1	Is the Head at the Right End of the Prism
Q	Is the Flow Rate from the Left End to the Right End
L	Is the Length of the Flow Path
A	Is the Cross Sectional Area Perpendicular to the Direction of Flow

Figure 23.—Prism of porous material illustrating Darcy's law.

Therefore, Darcy's law can be written as

$$Q = C(h_2 - h_1). \qquad (32)$$

Another form of the conductance definition for horizontal flow in a prism is

$$C = TW/L \qquad (33)$$

where

T is transmissivity (K times thickness of the prism) in the direction of flow (L^2t^{-1}); and

W is the width of the prism (L).

Conductance is defined for a particular prism of material and for a particular direction. In an anisotropic medium characterized by three principal directions of hydraulic conductivity, the conductances of a prism in these three principal directions will generally differ.

If a prism of porous material consists of two or more subprisms in series--that is, aligned sequentially in the direction of flow, as shown in figure 24--and the conductance of each subprism is known, a conductance representing the entire prism can be calculated. The equivalent conductance for the entire prism is the rate of flow in the prism divided by the head change across the prism.

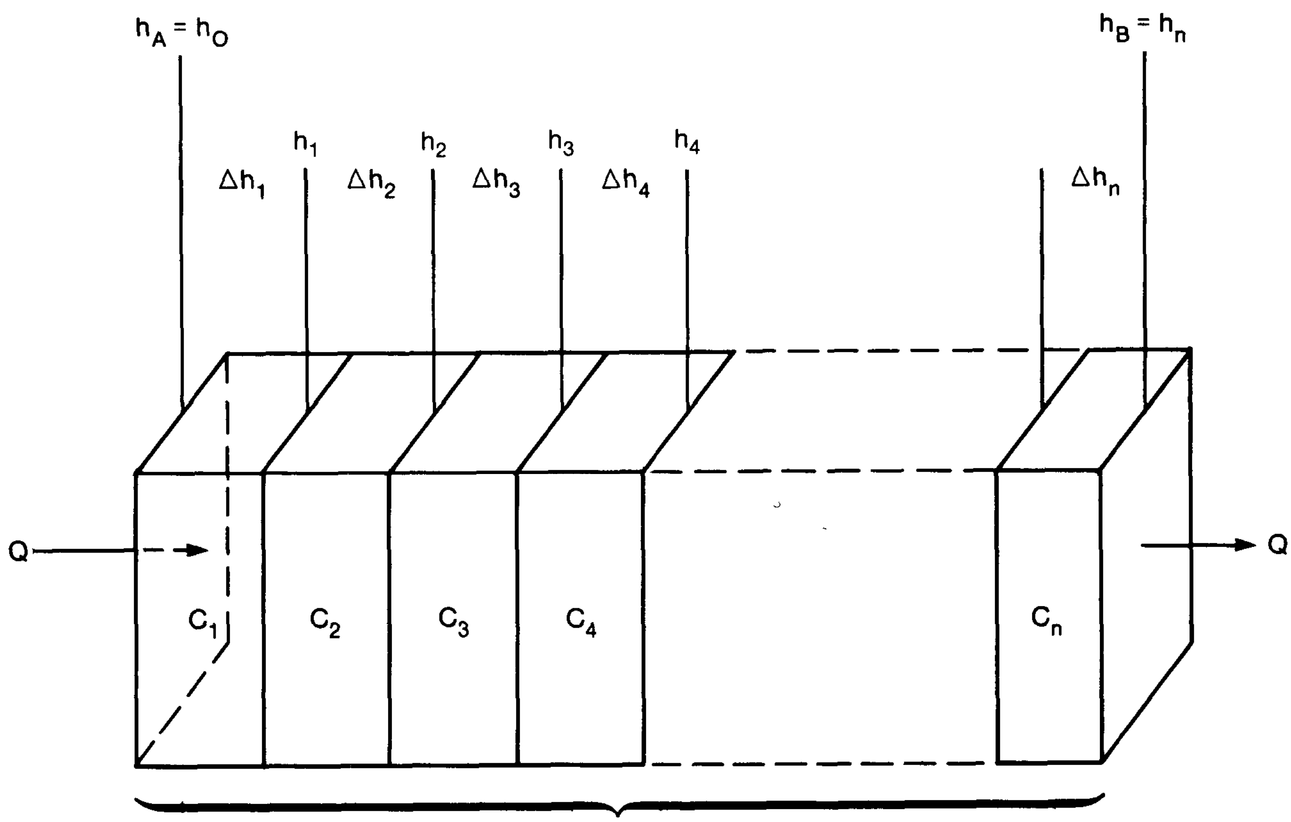
$$C = Q/(h_A - h_B) \qquad (34)$$

Assuming continuity of head across each section in series gives the identity

$$\sum_{i=1}^{n} \Delta h_i = h_A - h_B. \qquad (35)$$

Substituting for head change across each section using Darcy's law (equation (32)) gives

$$\sum_{i=1}^{n} \frac{q_i}{C_i} = h_A - h_B. \qquad (36)$$



$$\frac{1}{C} = \frac{1}{C_1} + \frac{1}{C_2} + \frac{1}{C_3} + \cdots + \frac{1}{C_n}$$

Explanation

Q	Is the Flow Rate
C_m	Is Conductance of Prism m
h_m	Is Head at the Right Side of Prism m
Δh_m	Is the Head Change Across Prism m
C	Is the Conductance of the Entire Prism

Figure 24.—Calculation of conductance through several prisms in series.

Since flow is one-dimensional and we are assuming no accumulation or depletion in storage, all q_i are equal to the total flow Q; therefore,

$$Q \sum_{i=1}^{n} \frac{1}{C_i} = h_A - h_B \text{ and } \frac{h_A - h_B}{Q} = \sum_{i=1}^{n} \frac{1}{C_i}. \qquad (37)$$

By comparison with equation (34), it can be seen that

$$\frac{1}{C} = \sum_{i=1}^{n} \frac{1}{C_i} . \qquad (38)$$

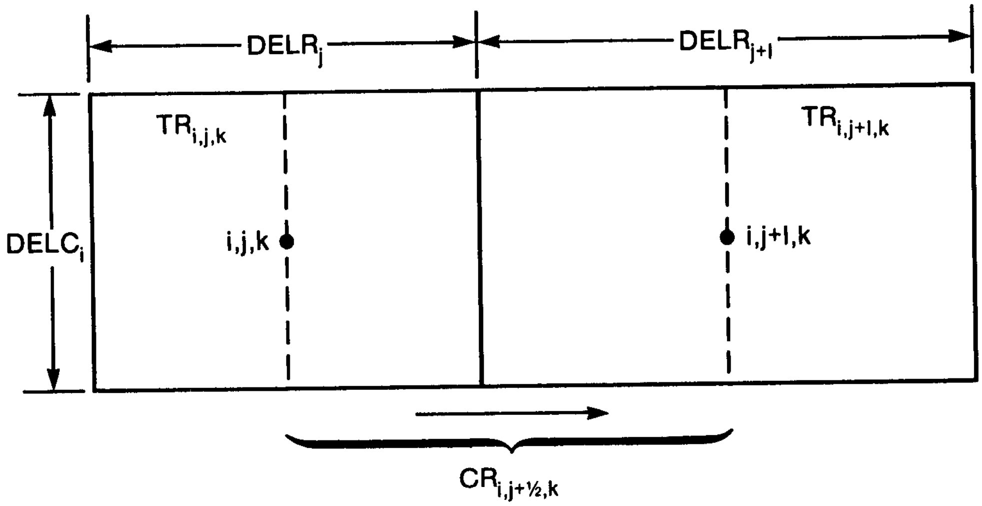
Thus for a set of conductances arranged in series, the inverse of the equivalent conductance equals the sum of the inverses of the individual conductances. When there are only two sections, the equivalent conductance reduces to

$$C = C_1 C_2 / (C_1 + C_2). \qquad (39)$$

Horizontal Conductance Under Confined Conditions

The finite-difference equations presented in this report use equivalent conductances between nodes of adjacent cells--i.e., "branch conductances,"--rather than conductances defined within individual cells. The horizontal conductance terms, CR and CC of equation (29), are calculated between adjacent horizontal nodes. CR terms are oriented along rows and thus specify conductance between two nodes in the same row. Similarly, CC terms specify conductance between two nodes in the same column. To designate conductance between nodes, as opposed to conductance within a cell, the subscript notation "1/2" is used. For example, $CR_{i,j+1/2,k}$ represents the conductance between nodes i,j,k and i,j+1,k.

Figure 25 illustrates two cells along a row, and the parameters used to calculate the conductance between nodes. Two assumptions are made: (1)



$$\frac{1}{CR_{i,j+\frac{1}{2},k}} = \frac{1}{\left(\dfrac{TR_{i,j,k}DELC_i}{\left(\dfrac{DELR_j}{2}\right)}\right)} + \frac{1}{\left(\dfrac{TR_{i,j+1,k}\,DELC_i}{\left(\dfrac{DELR_{j+1}}{2}\right)}\right)}$$

$$CR_{i,j+\frac{1}{2},k} = 2\,DELC_i \times \frac{TR_{i,j,k}\,TR_{i,j+1,k}}{TR_{i,j,k}\,DELR_{j+1} + TR_{i,j+1,k}\,DELR_j}$$

Explanation

$TR_{i,j,k}$ Is Transmissivity in the Row Direction in Cell i,j,k

$CR_{i,j+\frac{1}{2},k}$ Is Conductance in the Row Direction Between Nodes i,j,k and i,j+1,k

Figure 25.—Calculation of conductance between nodes using transmissivity and dimensions of cells.

the nodes are in the center of the cells and (2) the transmissivity is uniform over each cell. Thus the conductance between the nodes is the equivalent conductance of two half cells in series (C_1 and C_2). Applying equation (39) gives

$$CR_{i,j+1/2,k} = C_1 C_2/(C_1 + C_2). \qquad (40)$$

Substituting the conductance for each half cell from equation (33) gives

$$CR_{i,j+1/2,k} = \frac{\dfrac{TR_{i,j,k}\,DELC_i}{1/2\ DELR_j}\ \dfrac{TR_{i,j+1,k}\,DELC_i}{1/2\ DELR_{j+1}}}{\dfrac{TR_{i,j,k}\,DELC_i}{1/2\ DELR_j} + \dfrac{TR_{i,j+1,k}\,DELC_i}{1/2\ DELR_{j+1}}}$$

where

TR is transmissivity in the row direction (L^2t^{-1});

DELR is the grid width along a row (L); and

DELC is the grid width along a column (L).

DELR and DELC are identical to the terms Δr and Δc, respectively, which were introduced in figure 4 and equation (3), Chapter 2. The new notation is introduced here to conform to the input of the Block-Centered Flow Package.

Simplification of the above expression gives the final equation

$$CR_{i,j+1/2,k} = 2\ DELC_i \frac{TR_{i,j,k}TR_{i,j+1,k}}{TR_{i,j,k}DELR_{j+1} + TR_{i,j+1,k}DELR_j}. \qquad (41)$$

The same process can be applied to the calculation of $CC_{i+1/2,j,k}$ giving

$$CC_{i+1/2,j,k} = 2\ DELR_j \frac{TC_{i,j,k}TC_{i+1,j,k}}{TC_{i,j,k}DELC_{i+1} + TC_{i+1,j,k}DELC_i} \quad (42)$$

where

TC is the transmissivity in the column direction (L^2t^{-1}). Equations (41) and (42) are used in the BCF Package to calculate the horizontal conductances between nodes within each layer of the model. However, where the transmissivity of both cells is zero, the conductance between the nodes in the cells is set equal to zero without invoking the equations.

Horizontal Conductance Under Water Table Conditions

In a model layer which is confined, horizontal conductance will be constant for the simulation. If a layer is unconfined or potentially unconfined, new values of horizontal conductance must be calculated as the head fluctuates. This is done at the start of each iteration. First, transmissivity is calculated as the product of hydraulic conductivity and saturated thickness; then conductance is calculated from transmissivity and cell dimensions using equations (41) and (42).

Transmissivity within a cell in the row direction is calculated using one of the following three equations

if $HNEW_{i,j,k} \geq TOP_{i,j,k}$,

$$\text{then } TR_{i,j,k} = (TOP_{i,j,k} - BOT_{i,j,k})\ HYR_{i,j,k}; \quad (43)$$

if $TOP_{i,j,k} > HNEW_{i,j,k} > BOT_{i,j,k}$,

$$\text{then } TR_{i,j,k} = (HNEW_{i,j,k} - BOT_{i,j,k})\ HYR_{i,j,k}; \quad (44)$$

if $HNEW_{i,j,k} \leq BOT_{i,j,k}$,

then $TR_{i,j,k} = 0$ (45)

where

$HYR_{i,j,k}$ is the hydraulic conductivity of cell i,j,k in the row direction (Lt^{-1}); (this notation is introduced here to conform to the input of the Block-Centered Flow Package);

$TOP_{i,j,k}$ is the elevation of the top of cell i,j,k (L); and

$BOT_{i,j,k}$ is the elevation of the bottom of cell i,j,k (L).

Transmissivity in the column direction is the product of transmissivity in the row direction and a horizontal anisotropy factor specified by the user; the horizontal anisotropy factor is a constant for each layer. Conductances in each direction are calculated from transmissivity and cell dimensions. When head drops below the aquifer bottom (equation (45)), the cell is considered to be dewatered, and is permanently set to no flow; the model has no provision for the resaturation of a dewatered cell. Thus errors may arise in attempts to simulate situations in which actual reversals in water-level occur. Errors can also arise if oscillations of computed heads occur during iteration; if such computational oscillations cause head to drop erroneously below the botton of the cell, the cell will change to no flow for all succeeding iterations and time steps. As a means of controlling this problem, the iterative solvers contain provisions for slowing the rate of convergence.

In the program described herein a layer-type flag, LAYCON, is used to specify whether or not the simulation of water table conditions through equations (43)-(45) is to be invoked. This is discussed more fully in the section on data requirements.

Vertical Conductance Formulation

Vertical conductance terms are calculated within the model using data from an input array which incorporates both thickness and vertical hydraulic conductivity in a single term, and using horizontal (or map) areas calculated from cell dimensions. In general, the vertical interval between two nodes, i,j,k and and i,j,k+1, may be considered to contain n geohydrologic layers or units, having vertical hydraulic conductivities $K_1, K_2 \ldots . K_n$ and thicknesses Δz_1, $\Delta z_2 \ldots . \Delta z_n$. The map area of the cells around nodes i,j,k and i,j,k+1 is $DELR_j*DELC_i$; the vertical conductance of an individual geohydrologic layer, g, in this area is given by

$$C_g = \frac{K_g \, DELR_j*DELC_i}{\Delta z_g} \qquad (46)$$

The equivalent vertical conductance, $C_{i,j,k+1/2}$, for the full vertical interval between nodes i,j,k and i,j,k+1 is found by treating the n individual geohydrologic layers as conductances in series; this yields

$$\frac{1}{C_{i,j,k+1/2}} = \sum_{g=1}^{n} \frac{1}{C_g} =$$

$$\sum_{g=1}^{n} \frac{1}{\dfrac{K_g DELR_j*DELC_i}{\Delta z_g}} = \frac{1}{DELR_j*DELC_i} * \sum_{g=1}^{n} \frac{\Delta z_g}{K_g} \qquad (47)$$

rearranging equation (47)

$$\frac{C_{i,j,k+1/2}}{DELR_j*DELC_i} = \frac{1}{\sum_{g=1}^{n} \dfrac{\Delta z_g}{K_g}} \qquad (48)$$

The quantity $\frac{C_{i,j,k+1/2}}{DELR_j*DELC_i}$ has been termed the "vertical leakance " and is designated $Vcont_{i,j,k+1/2}$ in this report; thus we have

$$Vcont_{i,j,k+1/2} = \frac{1}{\sum_{g=1}^{n} \frac{\Delta z_g}{K_g}} \qquad (49)$$

Vcont is the term actually used as input in the model described herein. That is, rather than specifying a total thickness and an equivalent (or harmonic mean) vertical hydraulic conductivity for the interval between node i,j,k and node i,j,k+1, the user specifies the term $Vcont_{i,j,k+1/2}$, which is actually the conductance of the interval divided by the cell area, and as such incorporates both hydraulic conductivity and thickness. The program multiples Vcont by cell area to obtain vertical conductance. The values of Vcont must be calculated or determined externally to the program; this is generally done through an application of equation (49). The Vcont values are actually read as the elements of a two-dimensional input array, $Vcont_{i,j}$, for each layer. Each value of $Vcont_{i,j}$ is the vertical leakance for the interval between cell i,j,k and cell i,j,k+1--that is, for the interval between the layer for which the array is read, and the layer below it. It follows that the Vcont array is not read for the lowermost layer in the model. Although values of Vcont are thus read into the model through a series of two-dimensional input arrays, the discussion in this section will continue to be given in terms of three-dimensional array notation, $Vcont_{i,j,k+1/2}$, to emphasize the fact that the Vcont values refer to the intervals between layers.

Figure 26 shows a situation in which nodes i,j,k and i,j,k+1 both fall within a single hydrogeologic unit, having a vertical hydraulic conductivity $K_{z\ i,j}$ which is uniform at least within the cell area. For this case, application of equation (49) yields

$$Vcont_{i,j,k+1/2} = \frac{K_{z\ i,j}}{\Delta z_{k+1/2}} \qquad (50)$$

where $\Delta z_{k+1/2}$, the vertical distance between nodes, is the sum of $\frac{\Delta v_k}{2}$ and $\frac{\Delta v_{k+1}}{2}$, in which Δv represents layer thickness as in figure 1. This situation might be found, for example, where several model layers are used to represent a single geohydrologic unit in order to provide greater vertical resolution.

Figure 27 shows a case in which two adjacent model layers are used to represent two vertically adjacent hydrogeologic units, so that nodes i,j,k and i,j,k+1 fall at the midpoints of these geohydrologic layers. Each layer is characterized by its own value of vertical hydraulic conductivity, which is again assumed to be uniform at least over the cell area. The expression for Vcont in this case becomes

$$Vcont_{i,j,k+1/2} = \frac{1}{\dfrac{(\Delta v_k)/2}{K_{z\ i,j,k}} + \dfrac{(\Delta v_{k+1})/2}{K_{z\ i,j,k+1}}} \qquad (51)$$

where Δv_k is the thickness of model layer k

Δv_{k+1} is the thickness of model layer k+1

$K_{z\ i,j,k}$ is the vertical hydraulic conductivity of the upper layer in cell i,j,k

$K_{z\ i,j,k+1}$ is the vertical hydraulic conductivity of the lower layer in cell i,j,k+1

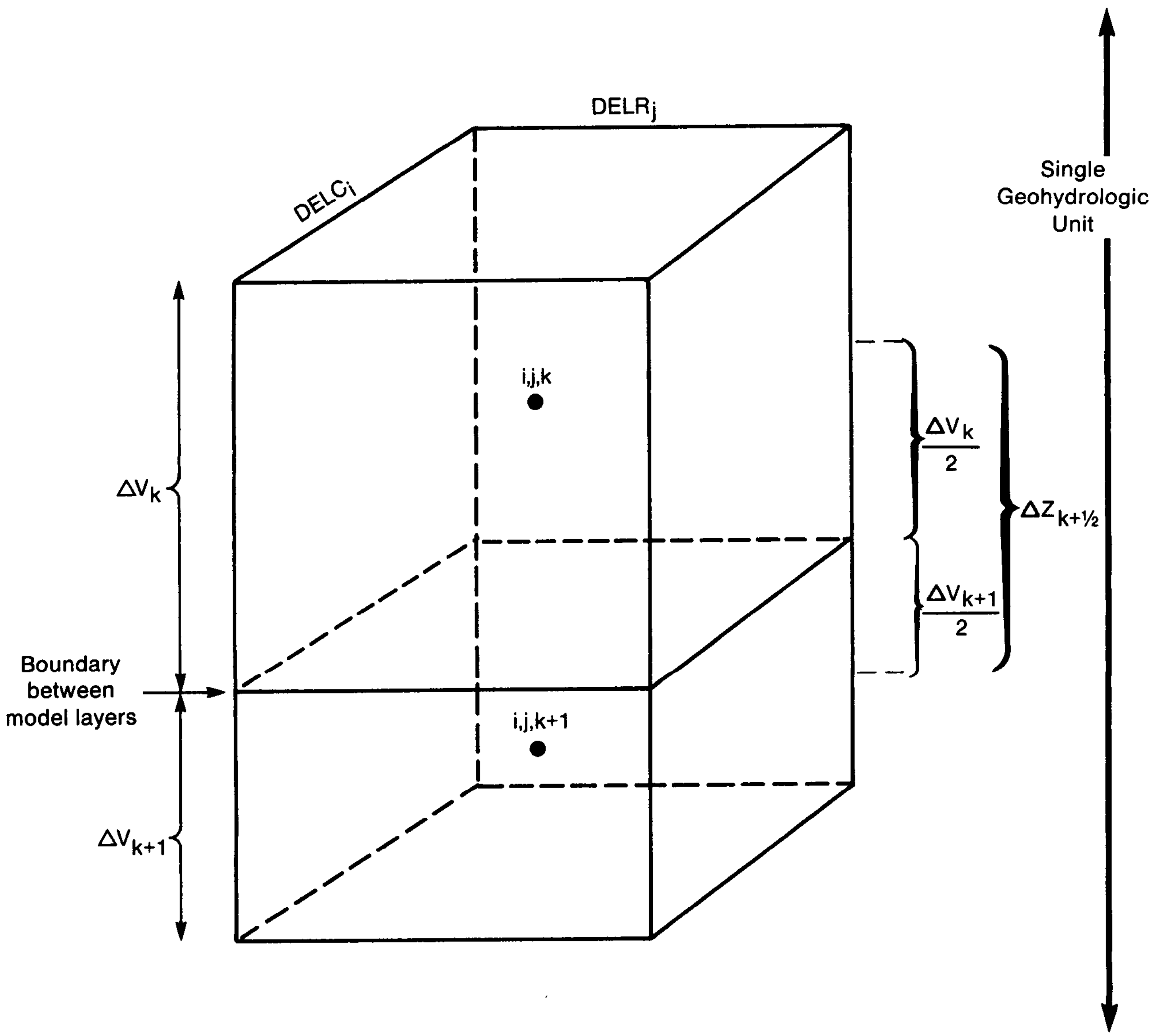


Figure 26.—Diagram for calculation of vertical leakance, Vcont, between two nodes which fall within a single geohydrologic unit.

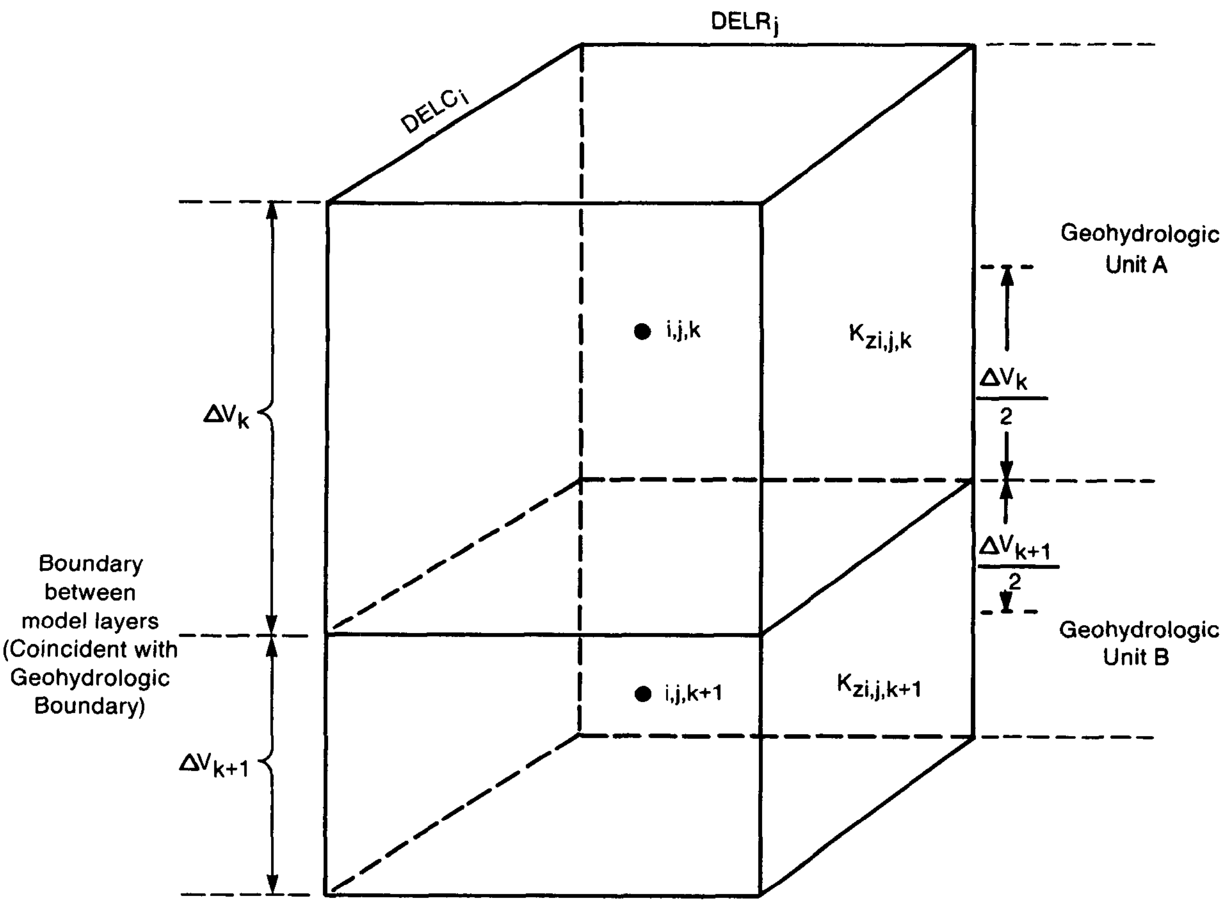


Figure 27.—Diagram for calculation of vertical leakance, Vcont, between two nodes located at the midpoints of vertically adjacent geohydrologic units.

If one value of K_z is much smaller than the other, the term containing the larger K_z value will be negligible in equation (51). Thus for this condition, only the term involving the smaller K_z value need be retained in the denominator of (51).

Figure 28 shows a third situation, in which node i,j,k and node i,j,k+1 are taken within (i.e., at the median depths of) two aquifers which are separated by a semiconfining unit. In this case, three intervals must be represented in the summation of equation (49)--the lower half of the upper aquifer, the semiconfining unit, and the upper half of the lower aquifer. The resulting expression for Vcont is

$$Vcont_{i,j,k+1/2} = \frac{1}{\frac{\Delta z_u/2}{K_{zu}} + \frac{\Delta z_c}{K_{zc}} + \frac{\Delta z_L/2}{K_{zL}}} \qquad (52)$$

where Δz_u is the thickness of the upper aquifer

Δz_c is the thickness of the confining bed

Δz_L is the thickness of the lower aquifer

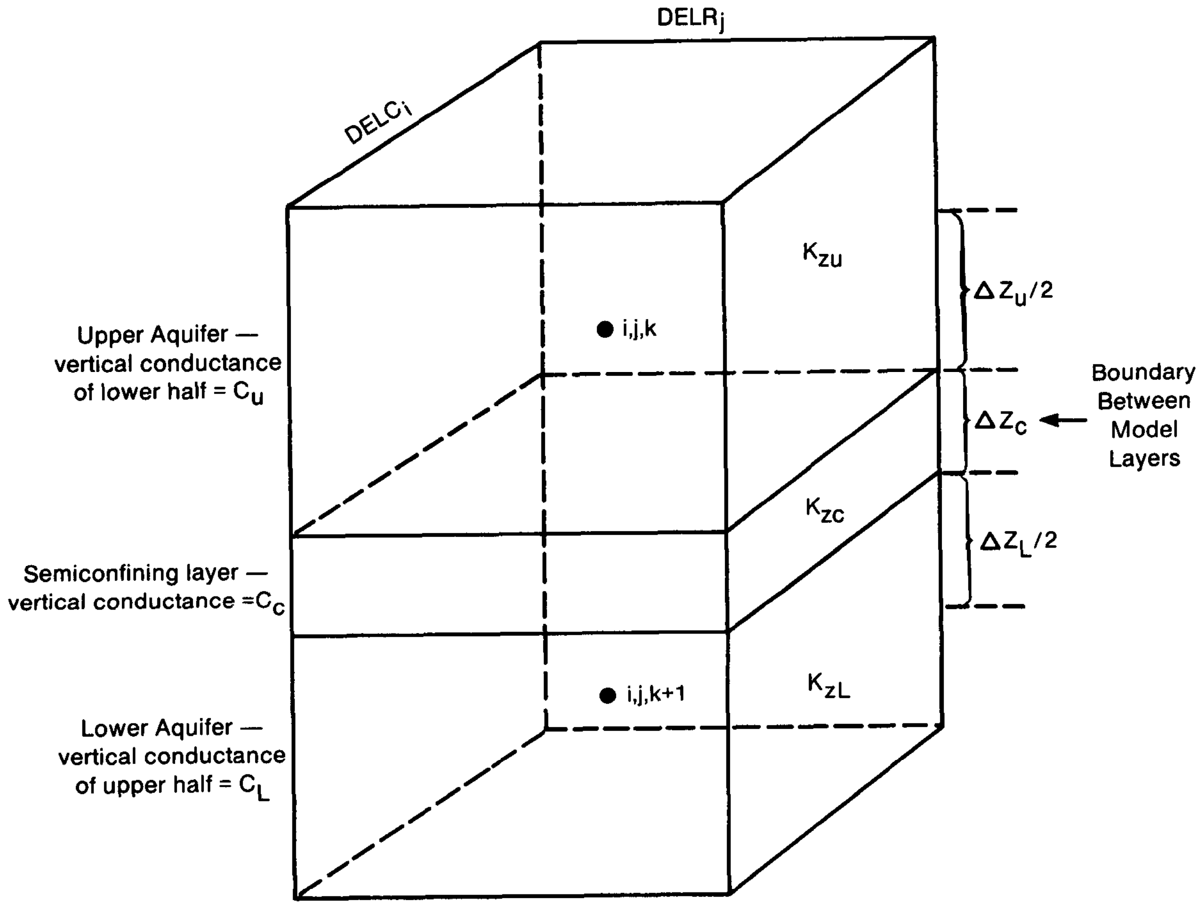
K_{zu} is the vertical hydraulic conductivity of the upper aquifer

K_{zc} is the vertical hydraulic conductivity of the semiconfining unit

K_{zL} is the vertical hydraulic conductivity of the lower aquifer; and

each of these terms must in general be considered to vary with the map location (i,j) of the nodes. In many applications it turns out that K_{zc} is much smaller than either K_{zu} or K_{zL}; in these situations the terms involving K_{zu} and K_{zL} are negligible in equation (52) so that the expression for Vcont becomes

$$Vcont_{i,j,k+1/2} = \frac{K_{zc}}{\Delta z_c} \qquad (53)$$



$$\frac{1}{C_{eq}} = \frac{1}{C_u} + \frac{1}{C_c} + \frac{1}{C_L} =$$

$$\frac{1}{DELC_i * DELR_j} \left\{ \frac{\Delta Z_u/2}{K_{zu}} + \frac{\Delta Z_c}{K_{zc}} + \frac{\Delta Z_L/2}{K_{zL}} \right\}$$

$$VCONT_{i,j,k+1/2} = \frac{1}{\frac{\Delta Z_u/2}{K_{zu}} + \frac{\Delta Z_c}{K_{zc}} + \frac{\Delta Z_L/2}{K_{zL}}}$$

Figure 28.—Diagram for calculation of vertical leakance, Vcont, between two nodes located at the midpoints of aquifers which are separated by a semiconfining unit.

If the formulation of equation (53) is applied to the situation shown in figure 28, and if the further assumptions are made that the confining bed makes no measureable contribution to the horizontal conductance or the storage capacity of either model layer, then in effect model layer k represents the upper aquifer, model layer k+1 represents the lower aquifer, and the confining bed is treated simply as the vertical conductance between the two model layers. This formulation is equivalent to that of figure 12, and is frequently referred to as the "quasi-three-dimensional" approach.

In summary, the model described herein utilizes a single input array, Vcont, which incorporates both vertical hydraulic conductivity and thickness, rather than independent inputs for thickness and conductivity. The program multiplies Vcont by cell area to obtain vertical conductance. This requires the user to calculate Vcont values externally to the program, using equation (49) in the general case (where n hydrogeologic layers occur in the vertical interval between nodes) or equations (50), (51), (52) or (53) in the situations shown in figures 26-28. While this approach involves some preprocessing of input data, it actually increases the flexibility of model application. Because layer transmissivity (or hydraulic conductivity and bottom elevation if unconfined) and layer storage coefficient are also used as input terms, the model never actually reads vertical gird spacing data. Thus the model can implement either the orthogonal mesh of figure 9-b or a deformed mesh such as that of figure 9-c, and can similarly be adapted to either a direct three-dimensional simulation or to the quasi-three-dimensional formulation, without modification of the program.

Vertical Flow Calculation Under Dewatered Conditions

The basic finite difference equation for cell i,j,k (equation (24)) was given as

$$CR_{i,j-1/2,k}(h^m_{i,j-1,k} - h^m_{i,j,k}) + CR_{i,j+1/2,k}(h^m_{i,j+1,k} - h^m_{i,j,k}) + CC_{i-1/2,j,k}(h^m_{i-1,j,k} - h^m_{i,j,k}) + CC_{i+1/2,j,k}(h^m_{i+1,j,k} - h^m_{i,j,k}) + CV_{i,j,k-1/2}(h^m_{i,j,k-1} - h^m_{i,j,k}) + CV_{i,j,k+1/2}(h^m_{i,j,k+1} - h^m_{i,j,k}) + P_{i,j,k}h^m_{i,j,k} + Q_{i,j,k} = SS_{i,j,k}(\Delta r_j \Delta c_i \Delta v_k) \frac{h^m_{i,j,k} - h^{m-1}_{i,j,k}}{t_m - t_{m-1}} \qquad (54)$$

In this equation the term $CV_{i,j,k+1/2}(h^m_{i,j,k+1} - h^m_{i,j,k})$ gives the flow into cell i,j,k through its lower face, i.e.

$$q_{i,j,k+1/2} = CV_{i,j,k+1/2}\,(h^m_{i,j,k+1} - h^m_{i,j,k}) \qquad (55)$$

where following the convention of equation (24), a positive value of $q_{i,j,k+1/2}$ indicates flow into cell i,j,k and a negative value indicates flow out of the cell. Equations (54) and (55) are based on the assumption that cells i,j,k and i,j,k+1 are fully saturated - i.e., that the water level in each cell stands higher than the elevation of the top of the cell. There are, however, situations in which a portion of a confined aquifer may become unsaturated--for example, when drawdown due to pumpage causes water levels to fall, at least locally, below the top of the aquifer. In terms of simulation, this condition is shown in figure 29. Two aquifers separated by a confining bed are simulated using the quasi-three-dimensional approach, in which the upper aquifer is represented by cell i,j,k, the underlying aquifer by cell i,j,k+1, and the confining bed by the vertical conductance between the two layers, $CV_{i,j,k+1/2}$. Pumping from the lower layer has

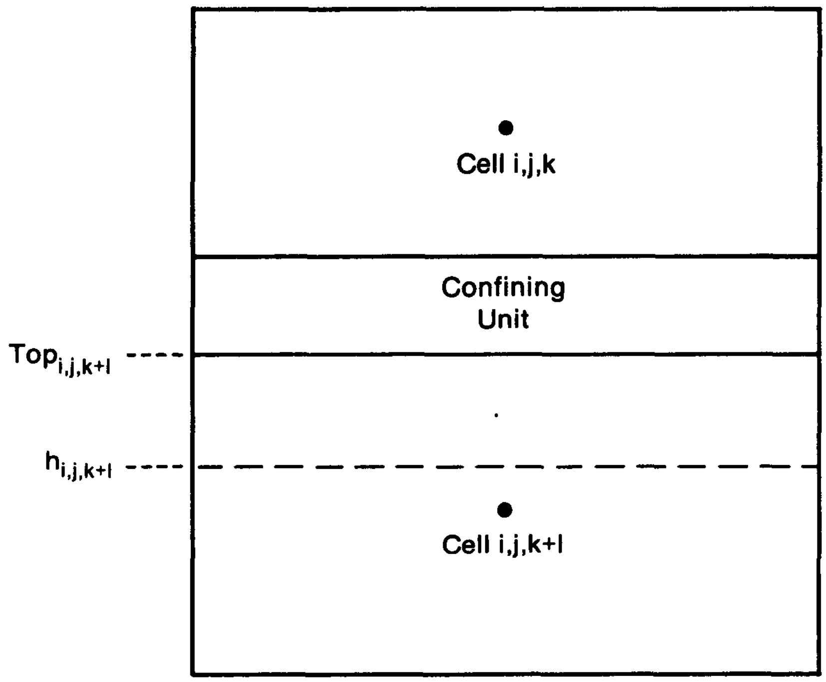


Figure 29.—Situation in which a correction is required to limit the downward flow into cell i,j,k+1, as a result of partial desaturation of the cell.

lowered the water level in cell i,j,k+1 below the elevation of the top of the cell, so that the aquifer is effectively unconfined within the cell area. An assumption is made that the confining layer remains fully saturated from top to bottom, and we consider the head difference across this confining unit. At the upper surface of the confining unit the head is simply that in the upper aquifer in cell i,j,k--$h_{i,j,k}$. Just below the lower surface of the confining unit, however, unsaturated conditions prevail, so that the pressure sensed on the lower surface of the confining unit is atmospheric--taken as zero in the model formulation. Thus the head at the base of the confining unit is simply the elevation at that point-i.e., the elevation of the top of the lower cell. If this elevation is designated $TOP_{i,j,k+1}$, the flow through the confining bed is obtained by substituting $TOP_{i,j,k+1}$ for $h_{i,j,k+1}$ in equation (55),

$$q_{i,j,k+1/2} = CV_{i,j,k+1/2}(TOP_{i,j,k+1} - h^{m}_{i,j,k}) \qquad (56)$$

Thus the flow will be downward, from cell i,j,k to cell i,j,k+1 (i.e., following the convention of equation (26), $q_{i,j,k+1/2}$ will be negative); but under this condition the flow will no longer be dependent on the water level, $h_{i,j,k+1}$, in the lower cell. The simplest approach to this probelm in formulating the equation for cell i,j,k would be to substitute the flow expression of equation (56) into equation (54), in place of the expression given in (55). However, if we consider the matrix of coefficients of the entire system of finite difference equations (matrix [A] of equation (27)), direct substitution of the expression in (56) into the equation for node i,j,k would render this matrix unsymmetric, generating problems in the solution process. To avoid this condition, an alternative approach is used. The flow term of equation (55) is allowed to remain on the left side of equation (54). The flow into cell i,j,k as computed by this term, is

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

(where in this case, since $h_{i,j,k} > h_{i,j,k+1}$, the computed flow is negative, indicating movement out of cell i,j,k.) The "actual" flow into cell i,j,k is given by equation (56) as $CV_{i,j,k+1/2}(TOP_{i,j,k+1} - h^m_{i,j,k})$ (where again $h^m_{i,j,k} > TOP_{i,j,k+1}$ indicating movement out of the cell). A correction term, q_c, can be obtained by subtracting equation (56) from equation (55), i.e.

$$q_c = \text{(computed flow into cell i,j,k)} - \text{("actual" flow into all i,j,k)} = CV_{i,j,k+1/2}(h^m_{i,j,k+1} - TOP_{i,j,k+1}) \quad (57)$$

To compensate for allowing the computed flow to remain on the left side of equation (54), the term q_c is added to the right side of equation (54). In the operation of the model, equation (54), which is identical to equation (24), is rearranged to the form of equation (26); and in practice, the term q_c is added to the right side, RHS, of equation (26). This immediately introduces a difficulty, since q_c contains the term $h^m_{i,j,k+1}$, and all terms involving unknown heads must be kept on the left side of equation (26). to circumvent this difficulty, q_c is actually computed using the value of $h^m_{i,j,k+1}$ from the preceding interation, rather than that from the current iteration, i.e.

$$q_{c,n} = CV_{i,j,k+1/2}(h^{m,n-1}_{i,j,k+1} - TOP_{i,j,k+1}) \quad (58)$$

where $q_{c,n}$ is the value of q_c to be added to RHS in the n^{th} iteration, and $h^{m,n-1}_{i,j,k+1}$ is the value of $h^m_{i,j,k+1}$ from the preceding iteration, n-1. As convergence is approached the difference between $h^{m,n-1}_{i,j,k+1}$ and $h^{m,n}_{i,j,k+1}$ becomes progressively smaller, and the approximation involved in (58) thus becomes more accurate. In the first iteration of each time step, the initial trial value of $h_{i,j,k+1}$ is used in computing q_c.

The process described above is used in formulating the equations for cell i,j,k when the underlying cell, i,j,k+1, has "dewatered"-i.e., when the water level in i,j,k+1 has fallen below the top of the cell. A correction must also be applied in formulating the equations for the dewatered cell itself. To examine this correction, we now take cell i,j,k to be the dewatered cell, and we consider flow into i,j,k from the overlying cell, i,j,k-1. For this case, the computed flow into cell i,j,k from above is $CV_{i,j,k-1/2}(h^m_{i,j,k-1} - h^m_{i,j,k})$ whereas the "actual" flow into the cell is $CV_{i,j,k-1/2}(h^m_{i,j,k-1} - TOP_{i,j,k})$. The difference, computed minus "actual" flow, is thus $q_c' = CV_{i,j,k-1/2}(TOP_{i,j,k} - h^m_{i,j,k})$ where q_c' should be added to the right hand side of equation (54) or (26). From a programming point of view, the most efficient way to handle this correction is to add the term $CV_{i,j,k-1/2}$ to HCOF on the left side of equation (26), while adding the term $(CV_{i,j,k-1/2} \cdot TOP_{i,j,k})$ to the RHS term. Because HCOF forms part of the coefficient of $h^m_{i,j,k}$, which falls on the main diagonal of the coefficient matrix, this correction does not affect the symmetry of the coefficient matrix; at the same time, the problems entailed in placing an unknown head value on the right side of the equation are avoided.

In summary, whenever dewatering of a cell occurs, two corrections must be made--one in formulating equation (26) as it applies to the overlying cell, and one in formulating equation (26) as it applies to the dewatered cell itself. These two corrections are discussed separately above, in each case using the designation i,j,k to represent the cell for which equation (26) is formulated. It is important to keep in mind, however, that both corrections are applied in any dewatering event, and that the form of the corrections has been developed to preserve the symmetry of the coefficient matrix [A] of equation (27), and to maximize program efficiency.

In the program described herein, the user specifies whether or not the procedure for limiting vertical flow under dewatered conditions is to be implemented. This is done through the layer type-flag, LAYCON, as discussed in the section on data requirements.

Storage Formulation

In the formulation of storage terms, the program described herein distinguishes between layers in which storage coefficient values remain constant throughout the simulation, and those in which the storage coefficient may "convert" from a confined value to a water table value, or vice-versa, as the water level in a cell falls below or rises above the top of the cell. This distinction is made through the use of the layer flag, LAYCON, as described in the section on data requirements.

For a layer in which storage coefficient is to remain constant during the simulation, the storage formulation is based upon a direct application of the storage expression in equation (24) or (54). This expression, which applies to an individual cell, i,j,k, has the form

$$\frac{\Delta V}{\Delta t} = SS_{i,j,k} \left(\Delta r_j \Delta c_i \Delta v_k\right) \frac{h^m_{i,j,k} - h^{m-1}_{i,j,k}}{t_m - t_{m-1}} \qquad (60)$$

where $\frac{\Delta V}{\Delta t}$ is the rate of accumulation of water in the cell, and as such must appear on the right side of equation (24) or (54); $SS_{i,j,k}$ is the specific storage of the material in cell i,j,k; Δr_j, Δc_i and Δv_k are the cell dimensions; $h^{m}_{i,j,k}$ is the head in cell i,j,k at the end of time step m; $h^{m-1}_{i,j,k}$ is the head in cell i,j,k at the end of time step m-1; t_m is the time at the end of time step m; and t_{m-1} is the time at the end of time step m-1. In equation (26) the notation $SC1_{i,j,k}$ was introduced, where $SC1_{i,j,k} = SS_{i,j,k}\Delta r_j \Delta c_i \Delta v_k$. In this report the term $SC1_{i,j,k}$ is termed the "storage capacity" or the "primary storage capacity" of cell i,j,k; the "primary" designation is used to distinguish $SC1_{i,j,k}$ from a secondary storage capacity which is used when storage term conversion is invoked, as explained in the following section. Using the concept of storage capacity, the expression for rate of accumulation in storage in cell i,j,k can be written

$$SC1_{i,j,k}(h^{m}_{i,j,k} - h^{m-1}_{i,j,k})/(t_m - t_{m-1}) \quad .$$

This expression is separated into two terms in equation (26), $SC1_{i,j,k}\, h^{m}_{i,j,k}/(t_m - t_{m-1})$, which is incorporated in the left side of (26) through the term $HCOF_{i,j,k}$, and $SC1_{i,j,k}\, h^{m-1}_{i,j,k}/(t_m - t_{m-1})$, which is included in the term $RHS_{i,j,k}$ on the right side of (26).

The input to the Block-Centered Flow Package requires specification of dimensionless storage coefficient values in each layer of the model; for a confined layer these storage coefficient values are given by the specific storage of the cell material multiplied by layer thickness in the cell, $SS_{i,j,k}\,\Delta v_k$; for an unconfined layer they are equal to the specific yield of the material in the cell. The incorporation of layer thickness into the confined storage term maintains the flexibility of the program to represent layers of varying thickness, and to implement either the direct three-dimensional or "quasi-three-dimensional" conceptualizations of vertical discretization. The storage coefficient values are read layer by layer; they are designated as array sf1 in the input instructions. These values are then multiplied by the cell areas, $\Delta r_j \Delta c_i$, to create storage capacity values, and they are stored in the SC1 array.

Storage Term Conversion

The primary storage capacity described above, $SC1_{i,j,k}$ is adequate for simulations in which the water level in each individual cell remains either above the top of the cell or below the top of the cell throughout the course of the simulation. If the water level crosses the top of a cell during a simulation--i.e., if the water level in a confined (fully saturated) cell falls below the top of the cell as a result of simulated pumpage, or if the water level in an unconfined cell rises above the top of the cell--then in effect the system "converts" from confined to water table conditions, or vice versa, during the simulation. Where these conditions appear to be possible, the user may invoke storage term conversion for the entire layer through use of the layer-type flag. When this is done, the primary storage capacity, $SC1_{i,j,k}$ for any cell in the layer will represent the confined storage coefficient multiplied by cell area; a secondary storage capacity, $SC2_{i,j,k}$ is used to represent specific yield multiplied by cell area. Values of confined storage coefficient for each cell in the layer are read through the two-dimensional input array sf1. These confined storage