

CHAPTER 5

Internal Flow Packages

This chapter documents two packages that simulate internal flow in MODFLOW. The packages are Block-Centered Flow (BCF) and Layer-Property Flow (LPF). Only one internal flow package can be used in a particular simulation. Internally, both packages use identical conceptualization. The difference is in the input data specified by the user and the details of implementation. This chapter begins with a number of sections describing the common conceptualization used in both packages. Later sections describe each of these package in detail. The final section describes the Horizontal-Flow Barrier (HFB) Package, which can be used to supplement BCF or LPF.

An internal flow package as previously mentioned in Chapter 3 calculates the CV, CR, and CC conductance coefficients and the ground-water storage terms in the finite-difference flow (eq. 2-24):

$$\begin{aligned}
 & CR_{i,j-1/2,k} (h_{i,j-1,k}^m - h_{i,j,k}^m) + CR_{i,j+1/2,k} (h_{i,j+1,k}^m - h_{i,j,k}^m) \\
 & + CC_{i-1/2,j,k} (h_{i-1,j,k}^m - h_{i,j,k}^m) + CC_{i+1/2,j,k} (h_{i+1,j,k}^m - h_{i,j,k}^m) \\
 & + CV_{i,j,k-1/2} (h_{i,j,k-1}^m - h_{i,j,k}^m) + CV_{i,j,k+1/2} (h_{i,j,k+1}^m - h_{i,j,k}^m) \\
 & + P_{i,j,k} h_{i,j,k}^m + Q_{i,j,k} = SS_{i,j,k} (DELR_j DELC_i \Delta v_{i,j,k}) \frac{h_{i,j,k}^m - h_{i,j,k}^{m-1}}{t^m - t^{m-1}}.
 \end{aligned} \tag{5-1}$$

The m superscript indicates the time step. In equation 5-1, Δr has been replaced by $DELR$, and Δc has been replaced with $DELC$. These new names are the variables used in the model code. Also, the subscript for cell thickness, Δv , has been expanded from k to i,j,k to allow for a vertically distorted grid (also called a deformed mesh) as discussed in Chapters 2 and 4.

For solution, equation 5-1 is transformed into the following (eq. 2-26):

$$\begin{aligned}
 & CV_{i,j,k-1/2} h_{i,j,k-1} + CC_{i-1/2,j,k} h_{i-1,j,k} + CR_{i,j-1/2,k} h_{i,j-1,k} \\
 & + (-CV_{i,j,k-1/2} - CC_{i-1/2,j,k} - CR_{i,j-1/2,k} - CR_{i,j+1/2,k} - CC_{i+1/2,j,k} - CV_{i,j,k+1/2} + HCOF_{i,j,k}) h_{i,j,k} \\
 & + CR_{i,j+1/2,k} h_{i,j+1,k} + CC_{i+1/2,j,k} h_{i+1,j,k} + CV_{i,j,k+1/2} h_{i,j,k+1} = RHS_{i,j,k}.
 \end{aligned} \tag{5-2}$$

The storage terms are incorporated within the HCOF and RHS coefficients, and the m time-step superscript has been removed.

Basic Hydraulic Conductance Equations

The concept of hydraulic conductance (shortened to conductance in this report) is defined in Chapter 2. Conductance is reviewed here, including 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 (fig. 5-1) as

$$Q = \frac{KA(h_1 - h_2)}{L}, \tag{5-3}$$

where

- Q is the volumetric 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);
- $h_1 - h_2$ is the head difference across the prism parallel to flow (L); and
- L is the length of the prism parallel to the flow path (L).

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Conductance, C , is defined as

$$C = \frac{KA}{L} . \quad (5-4)$$

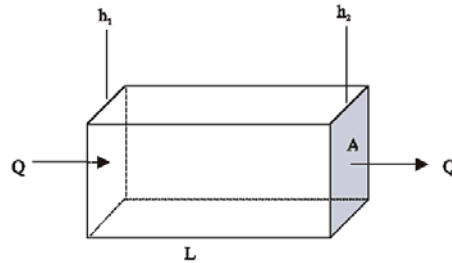


Figure 5-1. Prism of porous material illustrating Darcy's law. (From McDonald and Harbaugh, 1988.)

Therefore, Darcy's law can be written as

$$Q = C(h_1 - h_2) . \quad (5-5)$$

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

$$C = \frac{TW}{L} , \quad (5-6)$$

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 of flow. In an anisotropic medium that is 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 (aligned sequentially in the direction of flow) as shown in figure 5-2, 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:

$$C = \frac{Q}{h_A - h_B} . \quad (5-7)$$

Assuming continuity of head across each subprism gives the identity

$$\sum_{i=1}^n \Delta h_i = h_A - h_B , \quad (5-8)$$

substituting for head change across each subprism using Darcy's law (eq. 5-5) gives

$$\sum_{i=1}^n \frac{q_i}{c_i} = h_A - h_B, \quad (5-9)$$

where

q_i is the flow across subprism i , and
 c_i is the conductance of subprism i .

Because flow is one dimensional, and we assume no accumulation or depletion in storage, each q_i is equal to the total flow Q ; therefore,

$$Q \sum_{i=1}^n \frac{1}{c_i} = h_A - h_B \quad \text{and} \quad \frac{h_A - h_B}{Q} = \sum_{i=1}^n \frac{1}{c_i}. \quad (5-10)$$

By comparing equation 5-10 with equation 5-7, the reader can see that

$$\frac{1}{C} = \sum_{i=1}^n \frac{1}{c_i}. \quad (5-11)$$

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 only two subprisms exist, the equivalent conductance reduces to

$$C = \frac{c_1 c_2}{c_1 + c_2}. \quad (5-12)$$

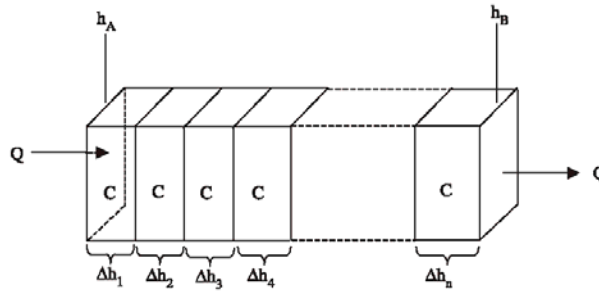


Figure 5-2. Calculation of conductance through several prisms in series. (From McDonald and Harbaugh, 1988.)

Horizontal Conductance

The finite-difference equations in MODFLOW use equivalent conductances between nodes of adjacent cells—that is, “branch conductances”—rather than conductances defined within individual cells. The horizontal conductance terms, CR and CC of equation 5-2, 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. (Remember that the “1/2” subscript denotes conductance between nodes, as opposed to conductance within a cell. For example, $CR_{i,j+1/2,k}$ represents the conductance between nodes i,j,k and $i,j+1,k$.)

An internal flow package reads data defining the horizontal hydraulic conductivity for individual cells and calculates conductance between nodes. Four methods of calculating these conductances are supported. The methods

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differ in the assumptions about the way the ground-water system varies from cell to cell. The four methods are described in the following two subsections.

Uniform Transmissivity within a Cell

The first method for computing horizontal conductance is based on the assumption that hydraulic conductivity times thickness, that is, transmissivity, is uniform within a cell. There can, however, be a discrete change in transmissivity at the boundary between any two cells. By use of this assumption and the previously mentioned assumption that nodes are in the center of cells, the conductance between the nodes is the equivalent conductance of two half cells in series. Figure 5-3 illustrates two cells along a row based on these assumptions. Substituting the conductance for each half cell (eq. 5-6) into equation 5-12 gives:

$$CR_{i,j+1/2,k} = \frac{\frac{TR_{i,j,k} DELC_i}{(\frac{1}{2})DELR_j} + \frac{TR_{i,j+1,k} DELC_i}{(\frac{1}{2})DELR_{j+1}}}{\frac{TR_{i,j,k} DELC_i}{(\frac{1}{2})DELR_j} + \frac{TR_{i,j+1,k} DELC_i}{(\frac{1}{2})DELR_{j+1}}} \quad (5-13)$$

where

$TR_{i,j,k}$ is transmissivity in the row direction at cell i,j,k (L^2T^{-1});

$DELR_j$ is the grid width of column j (L); and

$DELC_i$ is the grid width of row i (L).

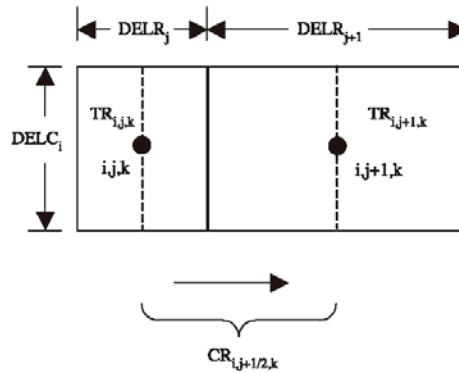


Figure 5-3. Calculation of conductance between nodes using transmissivities and dimensions of cells. (From McDonald and Harbaugh, 1988.)

Simplification of equation 5-13 gives the final equation:

$$CR_{i,j+1/2,k} = 2 DELC_i \frac{TR_{i,j,k} TR_{i,j+1,k}}{TR_{i,j,k} DELR_{j+1} + TR_{i,j+1,k} DELR_j} \quad (5-14)$$

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

$$CC_{i+1/2,j,k} = 2 DELR_j \frac{TC_{i,j,k} TC_{i+1,j,k}}{TC_{i,j,k} DELC_{i+1} + TC_{i+1,j,k} DELC_i} \quad (5-15)$$

where

$TC_{i,j,k}$ is the transmissivity in the column direction at cell i,j,k (L^2T^{-1}).

Equations 5-14 and 5-15 are used unless the transmissivity of both cells is zero, in which case the conductance between the nodes is set equal to zero without invoking the equations.

The above approach for calculating interblock conductance is called the “harmonic mean” method. The reason for this name can be seen by manipulating equation 5-14 into the following:

$$CR_{i,j+1/2,k} = \left(\frac{(\frac{1}{2})DEL R_j + (\frac{1}{2})DEL R_{j+1}}{\frac{(\frac{1}{2})DEL R_j}{TR_{i,j,k}} + \frac{(\frac{1}{2})DEL R_{j+1}}{TR_{i,j+1,k}}} \right) \frac{DEL C_i}{(\frac{1}{2})DEL R_j + (\frac{1}{2})DEL R_{j+1}} \quad (5-16)$$

The term in parentheses is the distance weighted harmonic mean of transmissivity of the two half cells, which by comparison with equation 5-6, can be seen to be the equivalent transmissivity between nodes i,j,k and $i,j+1,k$.

In order to apply the harmonic mean computation (eq. 5-14 and 5-15) for conductance between confined cells, transmissivity for each cell must be provided as input data or computed. Transmissivity is computed as

$$TR_{i,j,k} = \Delta v_{i,j,k} HK_{i,j,k} \quad (5-17A)$$

$$TC_{i,j,k} = \Delta v_{i,j,k} HK_{i,j,k} HANI_{i,j,k} \quad (5-17B)$$

where

$HK_{i,j,k}$ is the hydraulic conductivity of cell i,j,k in the row direction (LT^{-1});

$\Delta v_{i,j,k}$ is the saturated thickness of cell i,j,k (L); and

$HANI_{i,j,k}$ is the ratio of hydraulic conductivity along columns to the hydraulic conductivity along rows (dimensionless).

For confined cells, $\Delta v_{i,j,k}$ is simply the cell thickness (vertical cell width). This can be computed internally in MODFLOW using cell elevations in the discretization file:

$$\Delta v_{i,j,k} = (TOP_{i,j,k} - BOT_{i,j,k}) \quad (5-18)$$

where

$TOP_{i,j,k}$ 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).

For water-table conditions, $\Delta v_{i,j,k}$ depends on head. Further, a cell can convert between confined and water table within a simulation. The following approach for computing saturated thickness can be applied:

$$\text{if } HNEW_{i,j,k} \geq TOP_{i,j,k}, \quad \text{then } \Delta v_{i,j,k} = (TOP_{i,j,k} - BOT_{i,j,k}); \quad (5-19A)$$

$$\text{if } TOP_{i,j,k} > HNEW_{i,j,k} > BOT_{i,j,k}, \quad \text{then } \Delta v_{i,j,k} = (HNEW_{i,j,k} - BOT_{i,j,k}); \quad (5-19B)$$

$$\text{if } HNEW_{i,j,k} \leq BOT_{i,j,k}, \quad \text{then } \Delta v_{i,j,k} = 0. \quad (5-19C)$$

When water-table conditions are simulated, cell saturated thickness is recalculated at the start of each iteration using equation 5-19. Transmissivity values (TR and TC) are then calculated as the product of hydraulic conductivity, saturated thickness, and variable HANI (for TC) (eq. 5-17). Finally, conductance is recalculated using

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equations 5-14 and 5-15. If head drops below the aquifer bottom (eq. 5-19C), the cell is considered to be fully dewatered, and is set to no flow by changing $IBOUND_{i,j,k}$ to 0. The model also has provision for the resaturation of fully dewatered cells, which is described in another section of this report.

Three Alternative Approaches for Calculating Horizontal Branch Conductances

Goode and Appel (1992) discuss three alternative approaches for calculating the horizontal branch conductances. These alternative approaches are each based on different assumptions about the flow system: (1) transmissivity varies linearly between nodes; (2) the aquifer is flat and homogeneous with a water table; or (3) the aquifer is flat with a water table in which hydraulic conductivity varies linearly between nodes. For each approach, a formulation of interblock transmissivity is developed. The interblock conductance is then computed as the interblock transmissivity times cell width divided by distance between nodes according to equation 5-6.

When transmissivity varies linearly between nodes, the interblock transmissivity derived by Goode and Appel (1992) is:

$$\frac{T_2 - T_1}{\ln(T_2/T_1)}, \quad (5-20)$$

where T represents transmissivity and subscripts 2 and 1 indicate any two adjacent cells along a row or column. Transmissivity values for the cells are computed using equation 5-17 with equation 5-18 or 5-19 used for thickness. This is called the “logarithmic-mean” interblock transmissivity method. This formulation will produce exact solutions for steady-state, one-dimensional flow if flow is uniform and aligned with the direction of changing transmissivity. To save numerical effort, this function is approximated by

$$\frac{T_1 + T_2}{2} \text{ when } 0.995 \leq \frac{T_2}{T_1} \leq 1.005.$$

For an unconfined homogeneous aquifer with a flat bottom, the interblock transmissivity derived by Goode and Appel (1992) is:

$$\frac{T_1 + T_2}{2}. \quad (5-21)$$

Transmissivity values for the cells are computed using equation 5-17 with equation 5-18 or 5-19 used for thickness. This is called the “arithmetic-mean” interblock transmissivity method. This formulation will produce exact solutions for uniform, steady-state, one-dimensional flow.

For an unconfined aquifer with a flat bottom and with hydraulic conductivity varying linearly between nodes, Goode and Appel derive the interblock transmissivity as:

$$\left(\frac{\Delta v_1 + \Delta v_2}{2} \right) \left(\frac{K_1 - K_2}{\ln(K_2/K_1)} \right), \quad (5-22)$$

where K represents hydraulic conductivity. Thickness is computed with equation 5-18 or 5-19. This is called the “arithmetic-mean thickness and logarithmic-mean hydraulic conductivity” method. This formulation produces exact solutions for uniform, steady-state, one-dimensional flow when the hydraulic conductivity varies in the direction of flow. To save numerical effort, the hydraulic conductivity part of this function is approximated by $\frac{K_1 + K_2}{2}$ when

$$0.995 \leq \frac{K_2}{K_1} \leq 1.005.$$

Vertical Conductance

Vertical conductance is calculated assuming that nodes are in the center of cells and that discrete changes can occur in vertical hydraulic conductivity at layer boundaries. Figure 5-4 illustrates this situation for two cells in layers k and $k+1$. Under these assumptions, the vertical conductance between two nodes will be the equivalent conductance of two half cells in series. Substituting the conductance for each half cell from equation 5-4 into equation 5-11 gives

$$\frac{1}{CV_{i,j,k+1/2}} = \frac{1}{\frac{DEL R_j DEL C_i VK_{i,j,k}}{(\frac{1}{2})\Delta v_{i,j,k}}} + \frac{1}{\frac{DEL R_j DEL C_i VK_{i,j,k+1}}{(\frac{1}{2})\Delta v_{i,j,k+1}}} \quad , \quad (5-23)$$

where

$VK_{i,j,k}$ is vertical hydraulic conductivity of cell i,j,k and

$\Delta v_{i,j,k}$ is the saturated thickness of cell i,j,k as defined by equation 5-18 for confined cells and equation 5-19 for unconfined cells.

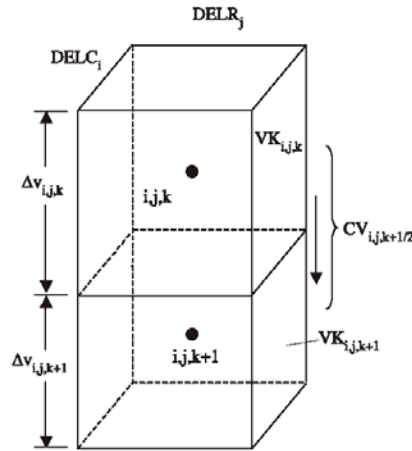


Figure 5-4. Calculation of vertical conductance between two nodes.
(Modified from McDonald and Harbaugh, 1988.)

Simplification of equation 5-23 gives

$$CV_{i,j,k+1/2} = \frac{DEL R_j DEL C_i}{\frac{(\frac{1}{2})\Delta v_{i,j,k}}{VK_{i,j,k}} + \frac{(\frac{1}{2})\Delta v_{i,j,k+1}}{VK_{i,j,k+1}}} \quad . \quad (5-24)$$

Figure 5-5 shows a second situation, in which cells i,j,k and $i,j,k+1$ are separated by a semiconfining unit. If the assumptions are made that the semiconfining unit makes no measurable contribution to the horizontal conductance or the storage capacity of either model layer, then the only effect of the confining bed is to restrict vertical flow between the model cells. Under these assumptions, the impact of the semiconfining unit can be simulated without using a separate layer in the finite-difference grid. This is done by including the semiconfining unit in the calculation of vertical conductance between the nodes. As mentioned previously, this is commonly referred to as the "Quasi-Three-Dimensional" (Quasi-3D) approach.

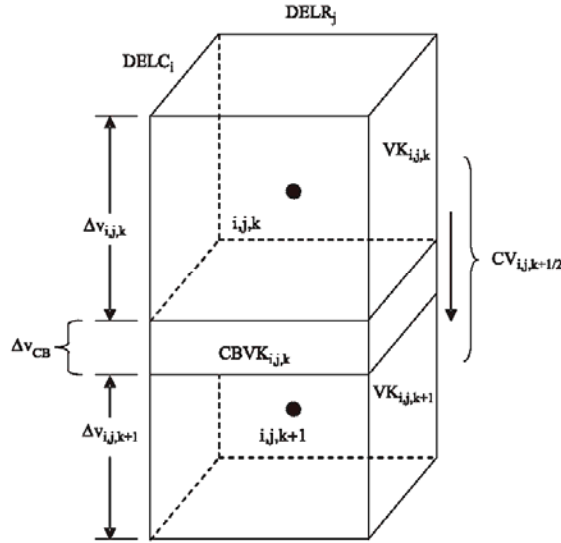


Figure 5-5. Calculation of vertical conductance between two nodes with a semiconfining unit between. (Modified from McDonald and Harbaugh, 1988.)

In the Quasi-3D approach, three intervals must be represented in the summation of conductance between the nodes—the lower half of the upper aquifer, the semiconfining unit, and the upper half of the lower aquifer. Equation 5-11 can be used to write an expression for the inverse of vertical conductance:

$$\frac{1}{CV_{i,j,k+1/2}} = \frac{1}{\frac{DELR_j DELC_i VK_{i,j,k}}{(\frac{1}{2})\Delta v_{i,j,k}}} + \frac{1}{\frac{DELR_j DELC_i VKCB_{i,j,k}}{\Delta v_{CB}}} + \frac{1}{\frac{DELR_j DELC_i VK_{i,j,k+1}}{(\frac{1}{2})\Delta v_{i,j,k+1}}} \quad (5-25)$$

where

$VKCB_{i,j,k}$ is the hydraulic conductivity of the semiconfining unit between cells i,j,k and $i,j,k+1$, and

Δv_{CB} is the thickness of the semiconfining unit.

Δv_{CB} is determined from information in the discretization file, and $VKCB_{i,j,k}$ is input data.

Simplification of equation 5-25 produces

$$CV_{i,j,k+1/2} = \frac{DELR_j DELC_i}{\frac{(\frac{1}{2})\Delta v_{i,j,k}}{VK_{i,j,k}} + \frac{\Delta v_{CB}}{VKCB_{i,j,k}} + \frac{(\frac{1}{2})\Delta v_{i,j,k+1}}{VK_{i,j,k+1}}} \quad (5-26)$$

Vertical Flow Correction Under Dewatered Conditions

This section describes the vertical flow correction capability that can be activated in both the BCF and LPF Packages. When this capability is activated, the vertical flow calculation is modified if a cell is unconfined (head is below its top elevation) while the cell directly above is fully or partially saturated. Such a situation can occur, for example, under perched conditions. The following paragraphs describe implementation of this capability. The sections on the BCF and LPF Packages describe the situations in which this capability is active.

From equation 5-1, the term that represents flow into cell i,j,k through its lower face, which will be called $q_{i,j,k+1/2}$, is

$$q_{i,j,k+1/2} = CV_{i,j,k+1/2} (h_{i,j,k+1} - h_{i,j,k}), \quad (5-27)$$

where the m superscript that indicates the time step has been removed. Following the convention of MODFLOW, 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. Equation 5-27 is based on the assumption that cells i,j,k and $i,j,k+1$ are fully saturated—that is, that the hydraulic head in each cell stands higher than the elevation of the top of the cell.

Situations can occur, however, in which part 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 an aquifer. This condition is most likely to occur when an aquifer is overlain by a lower conductivity unit. In terms of simulation, this condition is shown in figure 5-6. Cells in two model layers are represented. The upper cell (i,j,k) has lower hydraulic conductivity than the underlying cell ($i,j,k+1$), which represents an aquifer. Pumping from the lower layer has lowered the water level in cell $i,j,k+1$ below the elevation of the top of the cell; however, cell i,j,k remains fully saturated. Thus, cell $i,j,k+1$ is effectively unconfined even though the cell above is saturated.

Consider the calculation of flow between nodes in the upper and lower cells. In the upper cell, head is simply whatever head is at that cell— $h_{i,j,k}$. Just below the upper cell, 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 bottom of the upper cell is simply the elevation at that point—that is, the elevation of the top of the lower cell. If this elevation is designated $TOP_{i,j,k+1}$, then the actual flow through the confining bed is obtained by substituting $TOP_{i,j,k+1}$ for $h_{i,j,k+1}$ in equation 5-27,

$$q_{i,j,k+1/2} = CV_{i,j,k+1/2} (TOP_{i,j,k+1} - h_{i,j,k}). \quad (5-28)$$

Thus, the flow will be downward, from cell i,j,k to cell $i,j,k+1$, 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 problem in formulating the equation for cell i,j,k would be to substitute the flow expression of equation 5-28 into equation 5-1, in place of the expression given in equation 5-27. If we consider, however, the matrix of coefficients of the entire system of finite-difference equations, this direct substitution would render this matrix asymmetric, thus generating problems in the solution process.

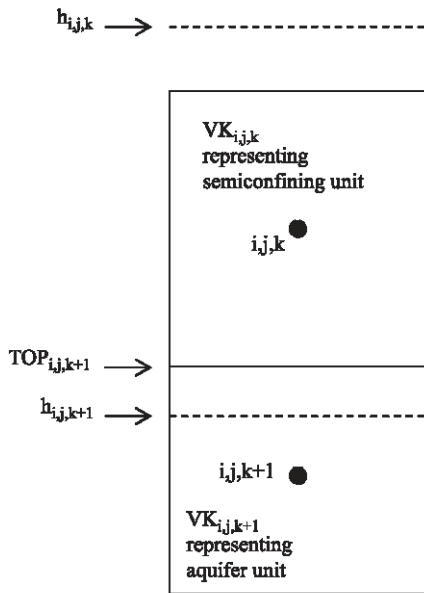


Figure 5-6. Situation in which a correction is required to limit the downward flow into cell $i,j,k+1$, as a result of partial desaturation of a cell. (From McDonald and Harbaugh, 1988.)

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To avoid this condition, an alternative approach is used. The flow term of equation 5-27 is allowed to remain on the left side of equation 5-1. The "actual" flow into cell i,j,k is given by equation 5-28, so a correction term, q_c , can be obtained by subtracting equation 5-28 from equation 5-27:

$$\begin{aligned} q_c &= (\text{computed flow into cell } i,j,k) - (\text{"actual" flow into cell } i,j,k) \\ &= CV_{i,j,k+1/2}(h_{i,j,k+1} - TOP_{i,j,k+1}) \end{aligned} \quad (5-29)$$

This correction term, q_c , should be added to the right side of equation 5-1 to compensate for allowing the computed flow to remain on the left side of equation 5-1. This again introduces a problem of matrix asymmetry because q_c contains the term $h_{i,j,k+1}$. To circumvent this difficulty, q_c is actually computed using the value of $h_{i,j,k+1}$ from the preceding iteration, rather than from the current iteration:

$$q_c^n = CV_{i,j,k+1/2}(h_{i,j,k+1}^{n-1} - TOP_{i,j,k+1}), \quad (5-30)$$

where

q_c^n is the value of q_c to be added to the right side of equation 5-2 in the n th iteration and

$h_{i,j,k+1}^{n-1}$ is the value of $h_{i,j,k+1}$ from the preceding iteration, $n-1$.

As convergence is approached, the difference between $h_{i,j,k+1}^{n-1}$ and $h_{i,j,k+1}^n$ becomes progressively smaller, and the approximation involved in equation 5-30 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 . In terms of equation 5-2, which is the form of the flow equation that is directly implemented in MODFLOW, q_c^n is added to $RHS_{i,j,k}$.

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"—that is, when the water level in $i,j,k+1$ has declined to below the top of the cell. A correction must also be applied in formulating the equations for the dewatered cell itself. To compute this correction, cell i,j,k is considered 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

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

whereas, the "actual" flow into the cell is

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

The difference, computed minus "actual" flow, is thus

$$q_c' = CV_{i,j,k-1/2}(TOP_{i,j,k} - h_{i,j,k}), \quad (5-31)$$

where q_c' is added to the right-hand side of equation 5-1. 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 5-2, while adding the term $CV_{i,j,k-1/2} TOP_{i,j,k}$ to the RHS term. This approach causes difficulties for some solution methods, however, because the dominance of the diagonal of the coefficient matrix of the finite-difference equations is reduced. So the same approach is used as described previously for the vertical correction for the cell above the dewatered cell. That is, q_c' is computed on the basis of the head from the previous iteration, and this correction is added to RHS of equation 5-2.

This conceptualization of limiting vertical flow also is valid when the unsaturated region in a lower layer is caused by an overlying confining unit that is simulated using the Quasi-3D approach. Although the confining unit is not simulated as a separate model layer when using this approach, the impact of the confining unit is still simulated through the vertical conductance calculation. The above vertical flow correction is applied with the value of $TOP_{i,j,k}$ being the bottom of the confining bed.

In summary, when the vertical flow correction capability is active, the correction applies whenever dewatering of a cell occurs below a cell that is not fully dewatered. The correction involves two adjustments—one in formulating equation 5-2 as it applies to the overlying cell, and one in formulating equation 5-2 as it applies to the dewatered cell itself. These two adjustments are discussed separately above, in each case using the designation i,j,k to represent the cell for which equation 5-2 is formulated. 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 of the finite-difference equations and its diagonal dominance.

Conversion from Dry Cell to Wet Cell

When saturated thickness is zero as defined by head being less than the bottom elevation of a cell (eq. 5-19C), it is clear that a variable-head (wet) cell should convert to dry. Unfortunately, there is not a straight-forward way to know when a dry cell should convert to wet. McDonald and others (1992) describe an approach for doing this and its application in the BCF Package of an earlier version of MODFLOW. The same approach is applied in MODFLOW-2005. The following is a brief overview of the approach. Readers should refer to McDonald and others (1992) for additional details. In particular, that report describes detailed information about numerical instabilities that can result from using this option, and several test problems are included.

A dry cell converts to wet based upon the head in an adjacent cell compared to a wetting threshold, THRESH, for the cell. If the head at the adjacent cell equals or exceeds the threshold at the start of a solution iteration, the dry cell is converted to wet. One option is to allow any of the four cells that are directly adjacent to the cell horizontally or the cell directly below to cause a dry cell to convert to wet are. Another option is to use only the cell below to determine when a dry cell becomes wet. The head below can be a better wetting indicator than the head at horizontally adjacent cells when the head variations between adjacent horizontal cells are larger than the vertical head variations, which is frequently the case.

A primary difficulty with this approach is that the value of THRESH must be determined by trial and error. If THRESH is too low, a cell may be incorrectly converted to wet. That is, a cell may convert to wet and then reconvert to dry in later solver iterations because the head does not stay above the bottom elevation. This cycle of converting between wet and dry conditions can repeat indefinitely, preventing the solver from converging. Larger values of THRESH can avoid repeated conversion between wet and dry, but they increase the non-uniqueness of the solution (McDonald and others, 1992, p. 8).

When a cell converts to wet, the initial estimate of head is established according to one of two equations:

$$h_{i,j,k} = \text{BOT}_{i,j,k} + \text{WETFCT}(h_n - \text{BOT}_{i,j,k}) \quad (5-32A)$$

or

$$h_{i,j,k} = \text{BOT}_{i,j,k} + \text{WETFCT}(\text{THRESH}_{i,j,k}), \quad (5-32B)$$

where

WETFCT is a user-specified constant, generally between 0 and 1, and

h_n is the head at the neighboring cell that causes cell i,j,k to convert to wet.

The user chooses the equation that works best for the problem being simulated. The initial estimate of head at a cell that converts to wet is theoretically unimportant because the solver should calculate the correct value in subsequent iterations. In practice, however, the initial estimate is often important for solver efficiency; that is, if a poor choice is made, the solver convergence may be slower than optimum. A bad choice for initial head also can cause the cell to oscillate between wet and dry.

Another user-specified option is the solver iteration interval for attempting to wet cells. For example, if the interval is 4, then cell wetting is attempted every 4 iterations. This can prevent the normal fluctuations in heads that can occur in iterative solvers in the next few iterations after cells are converted to wet from inappropriately triggering more cell wetting. All of these options are included to help make the solution process more stable. Refer to McDonald and others (1992) for more information about solution instability and how to deal with it.

Storage Formulation

A distinction is made in MODFLOW between confined layers in which storage terms remain constant throughout the simulation, and those layers in which the storage terms may "convert" from a confined value to a water-table value, or conversely from a water-table value to a confined value, as the water level in a cell falls below or rises above the top of the cell. For a confined layer, the storage formulation is based upon a direct application of the storage expression in equation 5-1. This expression for the rate of accumulation of water into a single cell is:

$$SS_{i,j,k} (DEL R_j DEL C_i \Delta v_{i,j,k}) \frac{h_{i,j,k}^m - h_{i,j,k}^{m-1}}{t^m - t^{m-1}} \quad (5-33)$$

where

- $SS_{i,j,k}$ is the specific storage of the material in cell i,j,k (L^{-1});
- $DEL R_j$ is the width of cells in column j (L);
- $DEL C_i$ is the width of cells in row i (L);
- $\Delta v_{i,j,k}$ is the cell thickness as defined by equation 5-18 (L);
- $h_{i,j,k}^m$ is the head in cell i,j,k at the end of time step m (L);
- $h_{i,j,k}^{m-1}$ is the head in cell i,j,k at the end of time step $m-1$ (L);
- t^m is the time at the end of time step m (T); and
- t^{m-1} is the time at the end of time step $m-1$ (T).

The notation $SC1_{i,j,k}$ is introduced where $SC1_{i,j,k} = SS_{i,j,k} (DEL R_j DEL C_i \Delta v_{i,j,k})$. 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. By using the concept of storage capacity, equation 5-33 can be rewritten as

$$SC1_{i,j,k} \frac{h_{i,j,k}^m - h_{i,j,k}^{m-1}}{t^m - t^{m-1}} \quad (5-34)$$

This expression is separated into two terms for inclusion into equation 5-2:

$$\frac{SC1_{i,j,k} h_{i,j,k}^m}{t^m - t^{m-1}},$$

which is incorporated in the left side of equation 5-2 through the term $HCOF_{i,j,k}$, and

$$\frac{-SC1_{i,j,k} h_{i,j,k}^{m-1}}{t^m - t^{m-1}},$$

which is included in the term $RHS_{i,j,k}$ on the right side of equation 5-2.

Storage Term Conversion

The primary storage capacity described above, $SC1_{i,j,k}$ is adequate for simulations in which a cell is confined throughout the course of a simulation; however, if the water level is below the top of a cell during a simulation, then the cell is under a water-table condition, and a different formulation for the rate of accumulation of water into a single cell applies:

$$SY(DELR_j DELC_i) \frac{h_{i,j,k}^m - h_{i,j,k}^{m-1}}{t^m - t^{m-1}}, \quad (5-35)$$

where

SY is the specific yield (dimensionless).

A secondary storage capacity, $SC2_{i,j,k}$, is used to represent specific yield multiplied by cell area, and equation 5-35 can be written as

$$SC2_{i,j,k} \frac{h_{i,j,k}^m - h_{i,j,k}^{m-1}}{t^m - t^{m-1}}. \quad (5-36)$$

During any one time step, four storage conditions are possible for each cell:

- The cell is confined for the entire time step,
- The cell is unconfined for the entire time step,
- The cell converts from confined to unconfined, and
- The cell converts from unconfined to confined.

The following expression for rate of accumulation in storage in cell i,j,k is used to handle all four possibilities:

$$\frac{SCB(h_{i,j,k}^m - TOP_{i,j,k}) + SCA(TOP_{i,j,k} - h_{i,j,k}^{m-1})}{t^m - t^{m-1}}, \quad (5-37)$$

where

TOP is the elevation of the top of the model cell,

SCA is the storage capacity in effect in cell i,j,k at the start of the time step; and

SCB is the "current" storage capacity—that is, the storage capacity in effect during the current iteration.

Equation 5-37 handles the four situations as follows. First, consider a case in which the head in cell i,j,k at the beginning of time step m ($h_{i,j,k}^{m-1}$) is above the top of the cell (fig. 5-7). Because no free surface exists in the cell at the start of the time step, the storage capacity at that time is taken as the confined storage capacity; that is, SCA is set equal to $SC1_{i,j,k}$. If, during a given iteration for time step m , the computed value of head for the end of the time step ($h_{i,j,k}^m$) is found to be above the top of the cell, then SCB for the following iteration also is set equal to $SC1_{i,j,k}$; equation 5-37 for that iteration then reverts to the form of equation 5-34, the equation for confined storage. If, however, the computed value of $h_{i,j,k}^m$ in a given iteration turns out to be below the top of the cell, as shown in figure 5-7, the value of SCB for the following iteration is set equal to $SC2$, the unconfined storage capacity. In this case, the computed rate of release of water from storage in the time step has two components:

$\frac{SC1_{i,j,k}(TOP_{i,j,k} - h_{i,j,k}^{m-1})}{t^m - t^{m-1}}$, the rate of release from confined or compressive storage, and

$\frac{SC2_{i,j,k}(h_{i,j,k}^m - TOP_{i,j,k})}{t^m - t^{m-1}}$, the rate of release from water-table storage.

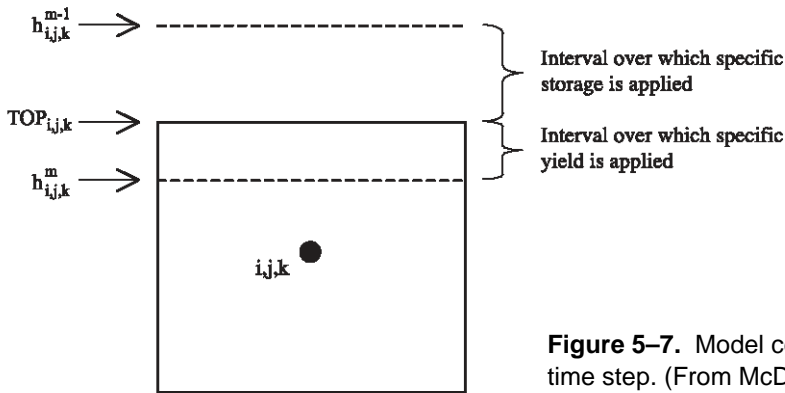


Figure 5-7. Model cell for which two storage factors are used during one time step. (From McDonald and Harbaugh, 1988.)

If the head at the beginning of the time step, $h_{i,j,k}$, is below the top of cell i,j,k , so that a free surface exists within the cell, SCA in equation 5-37 is set equal to $SC2_{i,j,k}$. If, during an iteration for time step m , the computed value of head for the end of the time step is below the top of the cell, SCB in the subsequent iteration is also set equal to $SC2_{i,j,k}$, and equation 5-37 reverts to the form of equation 5-36. If, however, the computed head for the end of the time step turns out to be above the top of the cell, SCB in the subsequent iteration is set equal to $SC1_{i,j,k}$, the confined storage capacity. This situation occurs during intervals of rising water level, and again two components are computed for the rate of accumulation of water in storage—one corresponding to unconfined or water-table storage and one corresponding to confined or compressive storage.

Equation 5-37 can be rearranged as follows:

$$\frac{SCB \times h_{i,j,k}^m}{t^m - t^{m-1}} + \frac{SCA(TOP_{i,j,k} - h_{i,j,k}^{m-1}) - SCB \times TOP_{i,j,k}}{t^m - t^{m-1}} \quad (5-38)$$

Equation 5-38 represents rate of accumulation in storage, which is the right side of equation 5-1. In the formulation of equation 5-2, therefore, the expression $\frac{SCB}{t^m - t^{m-1}}$ is subtracted from $HCOF_{i,j,k}$ on the left-hand side, while the term

$$\frac{SCA(TOP_{i,j,k} - h_{i,j,k}^{m-1}) - SCB \times TOP_{i,j,k}}{t^m - t^{m-1}}$$

is added to $RHS_{i,j,k}$ on the right-hand side.

Storage Formulation for Steady-State Simulations

For steady-state conditions, no storage effects exist; thus, nothing is added to RHS and HCOF coefficients to represent storage. A stress period can be specified as steady state in the discretization file. Normally, a steady-state

stress period will have a single time step. When all stress periods in a simulation are steady state, storage data are not included in the input data.

Applicability and Limitations of Optional Formulations

The options for calculation of horizontal conductance under water-table conditions, vertical flow correction, and storage term conversion were all developed on the assumption that each model layer corresponds to a distinct aquifer or permeable horizon, and that these horizons are separated by distinct units of low permeability. Use of these options where these conditions are not satisfied may lead to a variety of problems and inaccuracies in simulation. For example, if the option for horizontal conductance calculation under water-table conditions is used where a water-table aquifer is represented by several model layers, and the water table is expected to traverse more than one layer during simulation, incorrect conversion of cells to a no-flow condition may occur as iterations are carried out. If the wetting option is not used, conversion to no flow is irreversible. The wetting option allows conversion to no flow to be reversed, yet conversion back and forth can sometimes repeatedly occur so that solver convergence is not achieved. Thus, care should be exercised in the decision to use these options.

Block-Centered Flow Package

This section discusses the unique aspects of BCF, including the overall requirements for input data. The detailed input instructions are contained in Chapter 8.

BCF utilizes a layer-type code (LAYCON) to classify layers according to which of the head-dependent formulations are used. The user specifies the values of LAYCON for each layer. There are four possible values for LAYCON: 0 indicates a confined layer, 1 indicates a water-table layer, 2 indicates a limited convertible layer, and 3 indicates a fully convertible layer. Explanations for each value follow.

Layer-type 0 — Confined

In this category, all cells in the layer are assumed to have unchanging transmissivity throughout the simulation. The user must externally compute transmissivity in the row direction for cells, which is directly input into variable Tran, rather than having BCF compute transmissivity from cell thickness and hydraulic conductivity. Thus, the cell elevations in the discretization file are not used for computing transmissivity. Horizontal interblock conductance is computed from the user-specified transmissivities using the specified interblock transmissivity equation (for example equations 5-14 and 5-15 if harmonic mean is selected); however, the “arithmetic-mean thickness and logarithmic-mean hydraulic conductivity” method is not supported because that method requires cell hydraulic conductivity. Modification of transmissivity is not provided for as water level varies. If the simulation is transient, storage coefficient (the product of specific storage and cell thickness) is specified by the user in variable Sf1, and as with Tran, Sf1 must be computed outside of the model. Cell drying, cell wetting, storage term conversion, and vertical flow correction are not active. The conductance and storage terms are retained without change throughout the simulation.

This layer type normally is used to simulate confined conditions, but could also be used to simulate a layer in which unconfined conditions will always prevail, provided drawdowns are expected to be a small fraction of layer thickness and the vertical flow correction is not needed. If used to simulate an unconfined layer, specific yield should be entered in place of the confined storage coefficient.

Layer-type 1 — Unconfined

This layer type is utilized only in a single-layer model or in the uppermost layer of a model, and only where unconfined conditions are expected to persist in the layer throughout the entire period of simulation. Transmissivities are computed at each iteration as the products of hydraulic conductivity and saturated thickness values within the layer. There is no check to determine if the head exceeds the top elevation, so the thickness

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calculation includes only equations 5-19B and 5-19C. All four formulations for calculating horizontal interblock conductance are supported. Hydraulic conductivity is read into variable HY. Bottom elevations are determined from the elevations in the discretization file. If the simulation is indicated as transient, specific yield values are entered in the input variable Sf1. No provision is made for storage term conversion. Because use of this layer type would be inappropriate except in the uppermost layer, a check of the layer number is made whenever LAYCON is given a value of one; if the layer number is not also equal to 1, indicating the uppermost model layer, an error message is printed. Cell drying is active. Cell wetting can be activated as described below. Vertical flow correction does not apply because this layer type is only allowed for the top model layer.

Layer-type 2 — Limited Convertible

This layer type is used where heads may alternate between confined and unconfined conditions, so that storage term conversion and limitation of flow from above under dewatered conditions are both desirable. An assumption is made, however, that the saturated thickness will remain a high fraction of the layer thickness throughout the period of simulation, and accordingly transmissivity is not recalculated as the product of hydraulic conductivity and saturated thickness. Transmissivity values are entered in the variable Tran as they are for a confined layer (LAYCON 0). The “arithmetic-mean thickness and logarithmic-mean hydraulic conductivity,” but the other three methods for calculating horizontal interblock conductance are supported. For transient simulations, the storage term conversion option requires that both confined storage coefficient and specific yield be specified for each cell (variables Sf1 and Sf2, respectively). The vertical flow correction is active. The top elevation, which is required for the storage computations and vertical flow correction, is determined from elevation data in the discretization file. Cell drying and wetting are inactive.

Layer-Type 3 — Fully Convertible

This layer type incorporates all of the Block-Centered Flow options associated with water-table conditions. Transmissivities are recalculated at each iteration using hydraulic conductivity and layer top and bottom elevations, and both storage term conversion and vertical flow correction are implemented. The thickness calculation includes all three parts of equation 5-19. Confined storage coefficients are entered in the input variable Sf1, hydraulic conductivity values are then entered in the variable HY, and aquifer bottom and top elevations are determined from elevations in the discretization file. Specific yield values are entered in the variable Sf2. Cell drying is active, and wetting can be activated as described below. All four formulations for computing horizontal interblock conductance are supported.

Other BCF Conceptualizations

For all values of LAYCON, the user is required to enter vertical hydraulic conductivity divided by the flow distance (called vertical leakance) into variable VCONT. Within BCF, vertical leakance is multiplied by cell area to obtain vertical conductance. Vertical leakance for a layer represents the leakance between the nodes in that layer and the nodes in the next lower layer. For example, the VCONT values entered during the input sequence for layer 1 actually apply to the interval between the midpoint of layer 1 and the midpoint of layer 2. Accordingly, VCONT is not input for the bottom layer.

VCONT can be computed for the two conceptualizations presented in the Vertical Conductance Section by dividing the vertical conductance by cell area. When there is no Quasiv3D confining bed (eq. 5-24), the result is:

$$VCONT_{i,j,k+1/2} = \frac{1}{\frac{(1/2)\Delta v_{i,j,k}}{VK_{i,j,k}} + \frac{(1/2)\Delta v_{i,j,k+1}}{VK_{i,j,k+1}}} \quad (5-39)$$

When there is a Quasi-3D confining bed (eq. 5-26), the result is:

$$VCONT_{i,j,k+1/2} = \frac{1}{\frac{(\frac{1}{2})\Delta v_{i,j,k}}{VK_{i,j,k}} + \frac{\Delta v_{CB}}{VKCB_{i,j,k}} + \frac{(\frac{1}{2})\Delta v_{i,j,k+1}}{VK_{i,j,k+1}}} \quad (5-40)$$

Although in many situations one of these two conceptualizations will likely be desired, the approach in BCF of having vertical leakance specified as user input allows the user to compute vertical leakance using any desired conceptualization. Because vertical distance is incorporated in vertical leakance, BCF does not use cell elevations to determine vertical conductance. Vertical conductance remains constant throughout a simulation in BCF; therefore, vertical conductance is not modified when vertical flow is limited.

To reduce the amount of input data, the interblock transmissivity method is combined with the layer-type flag (LAYCON). The combined flag is called Ltype in the input instructions. The left digit of Ltype indicates the interblock transmissivity method and the right digit is the layer type. The interblock transmissivity values are:

- 0 indicates harmonic mean,
- 1 indicates arithmetic mean,
- 2 indicates logarithmic mean, and
- 3 indicates arithmetic-mean thickness and logarithmic-mean hydraulic conductivity.

For example, an Ltype value of 13 for a layer indicates arithmetic mean for interblock transmissivity and 3 for LAYCON.

A single IWDFLG variable for the entire grid determines whether the wetting capability (conversion of dry cells to wet) is active. Even when wetting is active, however, wetting will occur only in layers where LAYCON is 1 or 3. The user must specify variable WETDRY for every layer where LAYCON is 1 or 3. The wetting threshold is determined as the absolute value of WETDRY. Negative values of WETDRY indicate that wetting is based only on the head in the cell below. Positive values indicate that wetting is based on head from the four surrounding horizontal cells and the cell below. A zero value in WETDRY deactivates wetting for that cell.

Within each layer, the required hydraulic data must be specified for every cell, including constant-head and no-flow cells. For no-flow cells, the entered values are never used in calculation, and thus any values may be specified; for constant-head cells, the storage terms are not used but the other data values are, and realistic values for those cells must be entered. BCF does not support the parameter method (Chapter 8) for defining any input data.

As indicated in equations 5-17A and 5-17B, two values of transmissivity are required at each cell—one in the row direction and one in the column direction. To reduce input effort, only a single value of transmissivity or hydraulic conductivity (depending on LAYCON) is read for each cell, giving only the value in the row direction; the row-direction values are subsequently multiplied by an anisotropic factor to obtain the corresponding column-direction values. A single value of the anisotropic factor is specified by the user for each layer, through the one-dimensional variable TRPY (NLAY).

Layer-Property Flow Package

This section discusses the unique aspects of the LPF Package, including the overall requirements for input data. The detailed input instructions are contained in Chapter 8.

The LPF Package supports two types of layers – confined and convertible. A confined layer is one in which transmissivity is constant throughout the simulation. Transmissivity is computed from hydraulic conductivity and cell elevations using equations 5-18 and 5-17. In transient simulations, the storage flow is computed from specific storage. The cell drying, cell wetting, and vertical flow correction capabilities are not active.

A convertible layer is one in which transmissivity varies based on head throughout the simulation. Transmissivity is computed during each solver iteration based on cell thickness computed from equation 5-19. The computation of transmissivity includes the possibility for a cell converting to no flow when head goes below the

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bottom elevation. The vertical flow correction capability is active, and the cell wetting capability can be applied if desired.

For convertible layers, the storage contribution to the flow equation is determined from confined and/or unconfined storage, depending on head compared to the top elevation of cells. Values of specific storage for each cell in the layer are read through the variable *Ss*, and values of specific yield for each cell in the layer are read through the variable *Sy*. The specific-storage values are multiplied by cell volume to obtain confined storage capacity, and the specific-yield values are multiplied by cell area to obtain unconfined storage capacity. Thus, two storage capacities are stored, and the program uses the appropriate value, depending on head conditions at each iteration.

LPF supports the “harmonic mean,” “logarithmic mean,” and “arithmetic-mean and logarithmic-mean hydraulic conductivity” horizontal interblock transmissivity formulations. Because the “arithmetic-mean thickness and logarithmic-mean hydraulic conductivity” method reduces to the “arithmetic-mean” method when the aquifer is homogeneous, the “arithmetic-mean” method is not separately included in the LPF Package. That is, only equations 5-20 and 5-22 are included in the LPF Package along with the harmonic mean method.

As shown in equation 5-17A, the transmissivity in the row direction for a cell is computed as the product of the cell hydraulic conductivity and the saturated thickness. The row-direction values are subsequently multiplied by an anisotropic factor to obtain the corresponding column-direction values (eq. 5-17B). A single value of the anisotropic factor can be specified by the user for each layer through variable *CHANI*; or a layer can have one value of horizontal anisotropy for each cell in variable *HANI*.

In confined and convertible situations, vertical conductance is computed using equation 5-24 or 5-26, depending on whether a Quasi-3D confining bed exists. Vertical conductivity is required for all cells to allow vertical conductance to be computed. Vertical hydraulic conductivity can be directly specified as input data, or the ratio of horizontal to vertical hydraulic conductivity can be input. Further, the vertical conductance of the confining bed is required when the Quasi-3D approximation is used. In convertible layers, vertical conductance is recomputed every iteration. Also, vertical conductance is adjusted when the vertical flow correction is active. This adjustment removes the component of vertical conductance for the unconfined cell that is below a wet cell.

The computations for vertical conductance for convertible layers can cause numerical instabilities because the change in conductance can be quite large between successive solver iterations. Accordingly, two options have been incorporated to avoid solution instability. The first option, called *CONSTANTCV*, keeps vertical conductance constant throughout the simulation, even for convertible layers. Vertical conductance is calculated from the cell thickness rather than saturated thickness. The second option is called *NOCVCORRECTION*, which prevents adjustment of vertical conductance when the vertical flow correction is applied. Note that the *CONSTANTCV* option automatically invokes the *NOCVCORRECTION* option.

In LPF, the convertible formulation should be used if layer 1 represents a water table. Also, the elevation of the top of layer 1, which is specified in the Discretization File, should be higher than the water level will reach at any time in the simulation. This will result in the use of equation 5-19B for calculating saturated thickness. It is the user’s responsibility in this situation to check to see that the simulated water level has not exceeded the top elevation, which would trigger the use of equation 5-19C for calculating saturated thickness. A logical approach for specifying the top elevation for a layer-1 water table is to set it equal to land-surface elevation. That is, in most situations the water table is not expected to exceed land-surface elevation.

The water-table formulations based on saturated thickness for convertible layers (horizontal conductance, vertical conductance, cell drying and wetting) can result in solution instability (excessive iterations or failure to converge) when saturated thickness is thin or layers have a large slope. One way to deal with such a problem is to simulate a convertible layer as confined. Although this approach results in errors to the extent that the computed head results in a saturated thickness different from the confined thickness, repeated trial and error simulations can then be made in which model data are adjusted to cause saturated thickness to be close to the confined thickness.

Two difficulties occur when approximating a convertible layer as confined. One difficulty is that for confined layers, the storage term in the flow equation is based on specific storage as input data. But if the cells are really unconfined, then specific yield should be used for the storage computations. This requires a user to compute specific storage as specific yield divided by cell thickness. This computation is conceptually simple, but inconvenient to implement if cell thickness varies throughout a layer. In this version of LPF (Version 7), an option named *STORAGECOEFFICIENT* has been added to resolve this problem. When *STORAGECOEFFICIENT* is used, then

the specific storage input values are viewed as storage coefficients, which are comparable in concept to specific yield.

The second difficulty with treating convertible layers as confined is that a user frequently wants to rerun the model with different saturated thickness values. This can be done by modifying the top elevations of layers in the Discretization File; however, the top elevation for one layer is also the bottom elevation for another. For example, the top of layer 2 is the bottom of layer 1 (or the bottom of the confining bed below layer 1 if the Quasi-3D option is being used). One generally does not want the bottom elevations adjusted when using this approach. An option named THICKSTRT has been added to LPF to provide a resolve this difficulty. The THICKSTRT option in combination with a negative LAYTYP value causes the specified layers to be confined and to have the cell thickness for conductance calculations computed from initial head (variable STRT read by the Basic Package) minus the bottom elevation rather than top elevation minus bottom elevation. The user can therefore rerun the model with different values for the initial head. The cell thickness for storage calculations is still top elevation minus bottom elevation for these layers unless the STORAGECOEFFICIENT option as described above is used.

The optional formulations described above are controlled by option variables, which have one value for each layer; that is, the options can be turned on or off on a layer by layer basis. The option variables are:

LAYCBD—Quasi-3D confining bed flag (read as part of the Discretization File),
 LAYTYP—Layer-type flag,
 LAYAVG—Interblock transmissivity flag,
 CHANI—Horizontal anisotropic flag and value,
 LAYVKA—Vertical anisotropic flag, and
 LAYWET—Wetting flag.

The Quasi-3D confining bed flag (LAYCBD) indicates whether a layer is underlain by a confining bed that is simulated using the Quasi-3D approach. This determines how vertical conductance is calculated.

LAYCBD = 0—there is no Quasi-3D confining bed below the layer, so vertical conductance is calculated using equation 5-24.

LAYCBD \neq 0—there is a Quasi-3D confining bed below the layer, so vertical conductance is calculated using equation 5-26.

The layer-type flag (LAYTYP) indicates whether a layer is confined or convertible. This controls whether (1) saturated thickness varies with head, (2) storage term conversion is used, and (3) vertical flow from above is limited under dewatered conditions:

Layer-type flag = 0 – The layer is simulated as confined. For a layer of this type, there is no provision for modification of saturated thickness as head varies, for storage term conversion, or for limitation of vertical flow from above if the calculated hydraulic head falls below the top of the cell.

Layer-type flag >0 – The layer is simulated as convertible between confined and unconfined. When the calculated hydraulic head is below the top of the cell, all of the options associated with water-table conditions are implemented. Saturated thickness and transmissivity are recalculated at each iteration on the basis of head, and both storage term conversion and limitation of flow from above under dewatered conditions are implemented.

Layer-type flag <0 – The layer is simulated as convertible unless the THICKSTRT option is in effect. When THICKSTRT is in effect, a negative value of LAYTYP indicates that the layer is confined, and its saturated thickness will be computed as the initial head minus (variable STRT) the bottom elevation.

The Interblock transmissivity flag (LAYAVG) indicates the method used for calculating horizontal interblock conductance:

LAYAVG = 0—Harmonic mean transmissivity is used. This assumes that transmissivity is uniform within a cell, and that changes occur as discrete changes at cell boundaries.

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LAYAVG = 1—logarithmic mean transmissivity is used. This assumes that hydraulic conductivity varies linearly between nodes.

LAYAVG = 2—arithmetic-mean thickness and logarithmic-mean hydraulic conductivity are used. This is based on a water-table condition.

The horizontal anisotropic flag (CHANI) indicates whether horizontal anisotropy is constant for a layer, or can vary at each cell in a layer. In either case, the grid is assumed to be aligned with the principal directions of hydraulic conductivity.

CHANI \leq 0.0—Horizontal anisotropy can vary at each cell in the layer. A separate layer-data variable of the horizontal anisotropic values (HANI) will be read in the input data.

CHANI > 0.0—Horizontal anisotropy is constant for all cells in the layer. The anisotropy is the value of the flag. For example, set CHANI=1.0 for an isotropic layer.

The vertical anisotropic flag (LAYVKA) indicates the type of values that are specified in variable VKA.

LAYVKA = 0—Values of VKA are vertical hydraulic conductivity of the model layer.

LAYVKA \neq 0—Values of VKA are the ratio of horizontal hydraulic conductivity (along rows) to vertical hydraulic conductivity for the model layer.

The wetting flag (LAYWET) indicates whether the wetting capability is on or off.

LAYWET = 0—Wetting capability is off.

LAYWET \neq 0—Wetting capability is on for the layer. This is valid only if the layer-type flag indicates that the layer is convertible (LAYTYP is not 0).

Most of the data values that must be specified for the LPF Package are layer data, meaning that the data must be defined for all cells in one or more of the model layers. As used in the equations in this chapter that define the LPF formulations, the layer-data variables have three-dimensional subscripts, indicating that there are values for all layers; however, some of the variables do not always exist for all layers. The layers for which these layer variables exist are determined by the values in the abovementioned option variables. The layer-data variables defined for use by LPF are:

HK—horizontal hydraulic conductivity along rows,

HANI—Ratio of horizontal hydraulic conductivity along columns to hydraulic conductivity along rows,

VKA—Vertical hydraulic conductivity or the ratio of horizontal hydraulic conductivity along rows (HK) to vertical hydraulic conductivity,

VKCB—Vertical hydraulic conductivity of a confining bed below a layer,

Ss—specific storage,

Sy—specific yield, and

WETDRY—wetting threshold combined with a wetting flag.

The discretization data—time and space—required by the LPF Package to formulate the flow and storage terms are specified in the Basic Package Discretization File. All other data required by LPF are read from the LPF data file. The input instructions (Chapter 8) describe the details of how the LPF input data are read. All of the layer variables can be directly read, and variables HK, HANI, VKA, VKCB, Ss, and Sy also can be defined by using parameters. The same method of data definition (directly reading or using parameters) must be used for all the layers for a given variable—that is, a particular variable cannot be defined by combining direct reading and using parameters.

When layer variables are read directly, a value is read for every cell even if the value will not be used. For no-flow cells, the values of variables are never used in any calculation, and thus any values may be specified; for constant-head cells, the Ss, Sy, and WETDRY variables are not used but the other variables are. When variables are

defined by using parameters, a value is required for variable-head cells ($IBOUND > 0$) and constant-head cells ($IBOUND < 0$). If a value is not assigned at one or more variable- or constant-head cells, the program will print an error message and stop.

Horizontal Flow Barrier Package

The capability to simulate thin, vertical, and low-permeability geologic features (barriers) was previously added to MODFLOW with the introduction of the Horizontal Flow Barrier (HFB) Package (Hsieh and Freckleton, 1993). This package has been incorporated into MODFLOW-2005. Figure 5-8 (from Hsieh and Freckleton, 1993) shows a conceptualization of a model layer containing a low-permeability barrier. HFB adjusts the horizontal hydraulic conductance computed by the internal flow package to account for the barriers. HFB is not a complete internal flow package, but rather acts as a supplement to the BCF and LPF Packages.

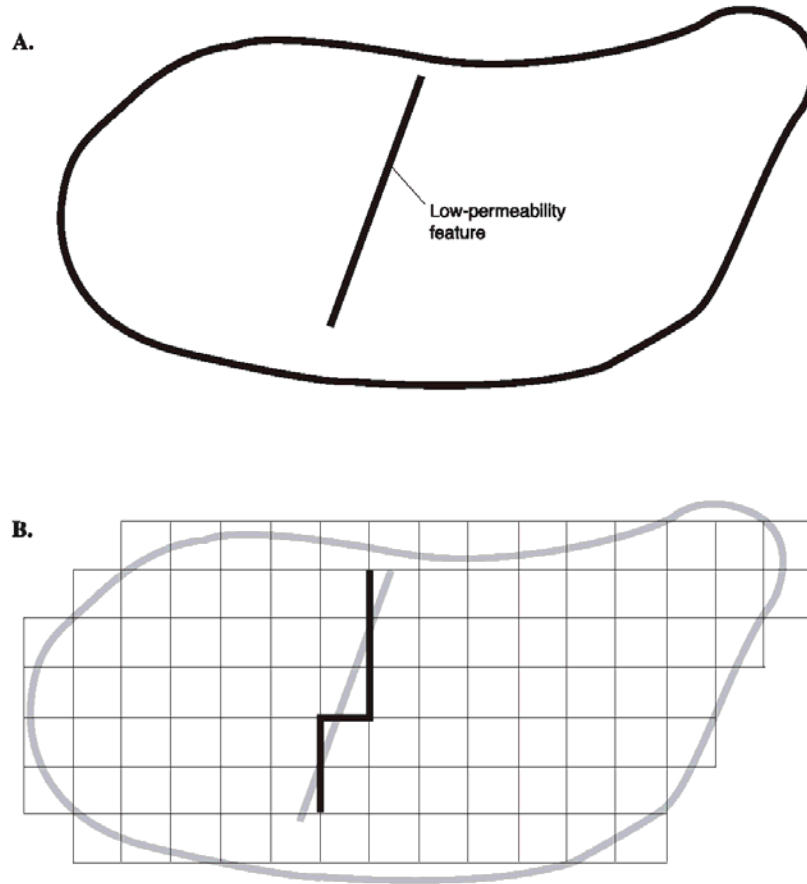


Figure 5-8. Schematic representation of (A) a model layer and (B) a grid with a low-permeability feature represented in the grid as a series of six horizontal-flow barriers. (From Hsieh and Freckleton, 1993.)

In the HFB Package, a barrier is conceptualized as being located on the boundary between two adjacent finite-difference cells in the same layer (fig. 5-9). The barrier is further conceptualized as being in series with the horizontal conductance computed by the internal flow package. Using equation 5-12, the equivalent conductance for the additional conductance of the barrier, C_{Barrier} , in series with the original cell conductance along a row, $CR_{i,j+1/2,k}^{\text{Original}}$, (fig. 5-9A) is:

$$CR_{i,j+1/2,k} = \frac{CR_{i,j+1/2,k}^{\text{Original}} C_{\text{Barrier}}}{CR_{i,j+1/2,k}^{\text{Original}} + C_{\text{Barrier}}} \quad (5-41)$$

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C_{Barrier} is computed by use of equation 5-4:

$$C_{\text{Barrier}} = \frac{K_{\text{Barrier}} \Delta v_{\text{Barrier}} \text{DELC}_i}{L_{\text{Barrier}}}, \quad (5-42)$$

where

- K_{Barrier} is hydraulic conductivity of the barrier,
- $\Delta v_{\text{Barrier}}$ is vertical thickness of the barrier, which is the average saturated thickness of the two cells, and
- L_{Barrier} is the distance across the barrier in the flow direction.

Conductance along a column is computed similarly. The distance across the barrier is assumed to be a small fraction of the distance between nodes so that the original conductance does not require correction because of the barrier. The HFB Package requires as input the “hydraulic characteristic” for a barrier, which is defined here as $K_{\text{Barrier}}/L_{\text{Barrier}}$. HFB includes the capability to use parameters to define the hydraulic characteristic. HFB does not simulate vertical barriers.

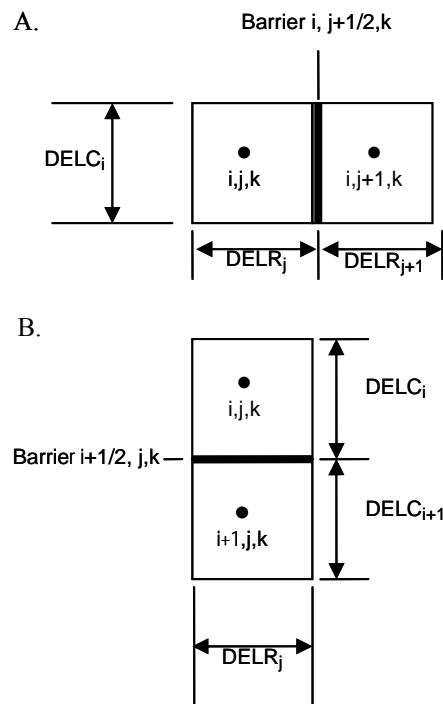


Figure 5-9. Schematic representation of a horizontal-flow barrier separating (A) two adjacent model cells in the same row and (B) two adjacent cells in the same column. (From Hsieh and Freckleton, 1993.)