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Chapter A3

A MODULAR FINITE-ELEMENT MODEL (MODFE) FOR AREAL AND AXISYMMETRIC GROUND-WATER-FLOW PROBLEMS, PART 1: MODEL DESCRIPTION AND USER'S MANUAL

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Book 6
MODELING TECHNIQUES

Although MICCG is an iterative method, values for iteration parameters are not input to MODFE. Instead, values for iteration parameters are computed automatically within the solver subroutine at the time of execution. Thus, with the appropriate value for the closure tolerance, TOL, the MICCG method will produce a solution efficiently that is as numerically accurate as the direct method.

Aquifer-Simulation Capabilities

MODFE contains the following aquifer-simulation capabilities:

- transient or steady-state conditions,
- nonhomogeneous and anisotropic flow where directions of anisotropy change within the model region,
- vertical leakage from a semiconfining layer that contains laterally nonhomogeneous properties and elastic storage effects,
- point and areally distributed sources and sinks,
- specified-head (Dirichlet), specified-flow (Neumann), and head-dependent (Cauchy-type) boundary conditions,
- vertical cross sections,
- axisymmetric-cylindrical flow,
- confined and unconfined (water-table) conditions,
- partial drying and resaturation of a water-table aquifer,
- conversion between confined- and unconfined-aquifer conditions,
- nonlinear-leakage functions (for simulating line, point, or areally distributed sources and sinks),
- changing stresses and boundary conditions on a stress-period basis, time-step basis, or both, and
- zoned input of hydraulic properties and boundary conditions.

The simulation capabilities listed above are described in sections of this report with regard to the physical processes that describe the hydrologic phenomena and to their implementation in MODFE. Mathematical symbols used by Cooley (1992) to describe these capabilities are replaced here by program variables which are contained in MODFE. Brief descriptions of data inputs for these simulation capabilities are given to enable the user to link the hydrologic phenomena to the mathematical representation in MODFE. Detailed data-input instructions are given in the section "Input Instructions."

Nonhomogeneity and Anisotropy

Two-dimensional ground-water flow in aquifers that exhibit nonhomogeneity and (or) anisotropy with regard to hydrologic characteristics (either hydraulic properties or boundary conditions) can be simulated by MODFE. Nonhomogeneous conditions are represented in MODFE by inputting distinct values for hydrologic characteristics by element or by node. The following hydrologic characteristics are input to MODFE by element:

- aquifer hydraulic conductivity or transmissivity,
- rotation angle for anisotropy in aquifer hydraulic conductivity or transmissivity,
- vertical hydraulic conductance of confining bed,
- aquifer storage coefficient and (or) specific yield, and
- unit rate of areally distributed stress.

The following hydrologic characteristics are input to MODFE by node:

- volumetric flow rates at point sources and sinks,
- aquifer thickness and altitude of aquifer top (for water-table simulations), and
- specified-flux, or head-dependent (Cauchy-type) flux boundary conditions (linear and nonlinear conditions).

Although MODFE can represent nonhomogeneity in hydrologic characteristics with element or nodal inputs, rarely are these characteristics known with enough detail throughout the aquifer region to permit the input of distinct values either by element or by node. Usually, values for hydrologic characteristics are generalized into zones, which contain either groups of elements or groups of element sides, from which element and nodal inputs can be obtained. A discussion of preparing data for input to MODFE by zone is given in the section "Hydraulic-Property and Boundary-Condition Zones."

Anisotropic flow, where principal values of hydraulic conductivity (or transmissivity) and principal directions vary within the aquifer region (fig. 9), can be represented by MODFE for simulation. Variation of principal values within the aquifer region is represented in the same manner as described above for nonhomogeneity; separate inputs are made for the principal values in the x and y directions by element or by zone. The program variables used to represent the principal values of transmissivity (or hydraulic conductivity) in the data input are XTR and YTR for the x and y directions, respectively. Details of these inputs by element or by zone are given in the section "Hydraulic-Property and Boundary-Condition Zones."

Anisotropic conditions of varying principal directions within the aquifer region are represented easily in MODFE by transforming the coordinates within elements that require change. The global x-y coordinate system that is used to represent nodal locations is rotated orthogonally within an element or a zone to a

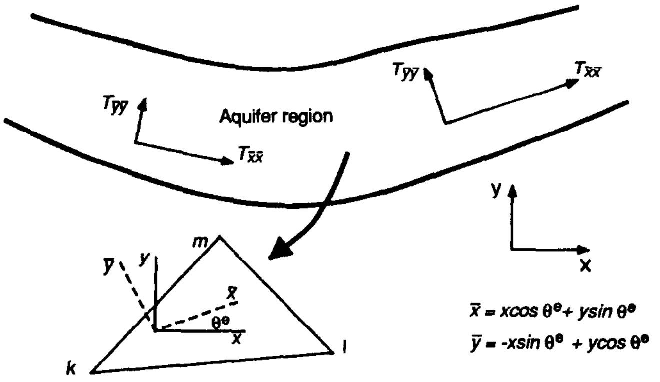


Figure 9.—Anisotropic flow conditions and nomenclature used to transform coordinates to local, $\bar{x}$-$\bar{y}$ system.

local $\bar{x}$-$\bar{y}$ system that coincides with the principal directions along which principal values of transmissivity (or hydraulic conductivity) have been determined. This transformation causes the symmetric transmissivity (or hydraulic conductivity) tensor of equation (1) to contain zero values for the off-diagonal or cross-product terms T_{xy} and T_{yx} (or K_{xy} and K_{yx}), and leaves the principal values $T_{\bar{x}\bar{x}}$ and $T_{\bar{y}\bar{y}}$ (or $K_{\bar{x}\bar{x}}$ and $K_{\bar{y}\bar{y}}$) in the tensor to characterize transmissivity (or hydraulic conductivity) in that part of the aquifer region. Usually, the principal values are determined by analyzing aquifer-test data. As described above, the principal values are input to MODFE by zone, and are represented by the program variables XTR and YTR for $T_{\bar{x}\bar{x}}$ ($K_{\bar{x}\bar{x}}$) and $T_{\bar{y}\bar{y}}$ ($K_{\bar{y}\bar{y}}$), respectively.

The rotation angle, θ^e, is the angular displacement of the local, $\bar{x}$-$\bar{y}$ system from the global x-y system, in degrees, measured counterclockwise. The rotation is performed automatically in MODFE by zone, according to the expressions shown in figure 9. If θ^e is zero, then no rotation is necessary. Because a zone could consist of only one element, it is possible to rotate elements individually. The rotation angle is represented in MODFE as the program variable ANG, and is input by zone along with the other zoned inputs listed above.

Steady Vertical Leakage

Steady vertical leakage through a confining bed from a source layer situated above or below an aquifer can be simulated by MODFE (fig. 10*A*). In addition to this application, steady vertical leakage can be used to represent leakage through the bottom of a wide, partially penetrating riverbed or lakebed, provided that the aquifer head is situated above the altitude of the bottom of the riverbed or lakebed (fig. 10*B*,*C*). (The condition in which the aquifer head sometimes lies below the altitudes of the bottom of an overlying confining bed and below the bottom of the riverbed or lakebed is represented in MODFE by a nonlinear leakage function, which is discussed in the section "Nonlinear-Leakage Functions"). The leakage is called steady because storage effects in the confining bed are not considered in the flow-rate computations; the flow rate from steady vertical leakage is dependent only on the vertical hydraulic conductance of the confining bed and on the head difference between the aquifer and the source layer. (The vertical leakage or yield of water stored elastically in a confining bed (transient leakage) is discussed in the following section.) Steady vertical leakage is represented in MODFE by the term $R(H - h)$ in equation (1), where R is vertical hydraulic conductance of the confining bed, H is source-layer head, and h is aquifer head (fig. 10).

Values of vertical hydraulic conductance are represented in MODFE by hydraulic-property zone, and are identified as the program variable VLC. Values for VLC can be computed from the zone representations of confining-bed thickness and vertical hydraulic conductivity. Usually, vertical hydraulic conductivity is not known with as much detail as is thickness; thus the aquifer region may contain only a few conductivity zones in comparison with the number of thickness zones. Preparation of zone inputs to MODFE are discussed in the section "Hydraulic-Property and Boundary-Condition Zones." Depending on the lithology and application of steady vertical leakage, the confining bed may consist of an entire geologic unit, several units, or part of one unit.

The source-layer head is input to MODFE by node, and is represented as the program variable HR. As shown in figure 10, the source-layer head can represent the head in an aquifer situated above or below the aquifer to be simulated, the head in a perched layer within the confining bed, or a lake or stream level.

The source-layer head, HR, may be changed with time during the simulation. Details of changing HR with time are given in the section "Changing Stresses and Boundary Conditions With Time."

Vertical Leakage of Water Stored Elastically in a Confining Bed

MODFE has the ability to simulate nonsteady vertical leakage of water stored elastically in a confining bed (transient leakage). The confining bed either can be an areally extensive geologic unit that completely or partially confines the simulated aquifer, or it can be a smaller unit, such as a riverbed or lakebed (fig. 10). Transient-leakage effects occur when nonsteady vertical hydraulic gradients are created and then dissi-

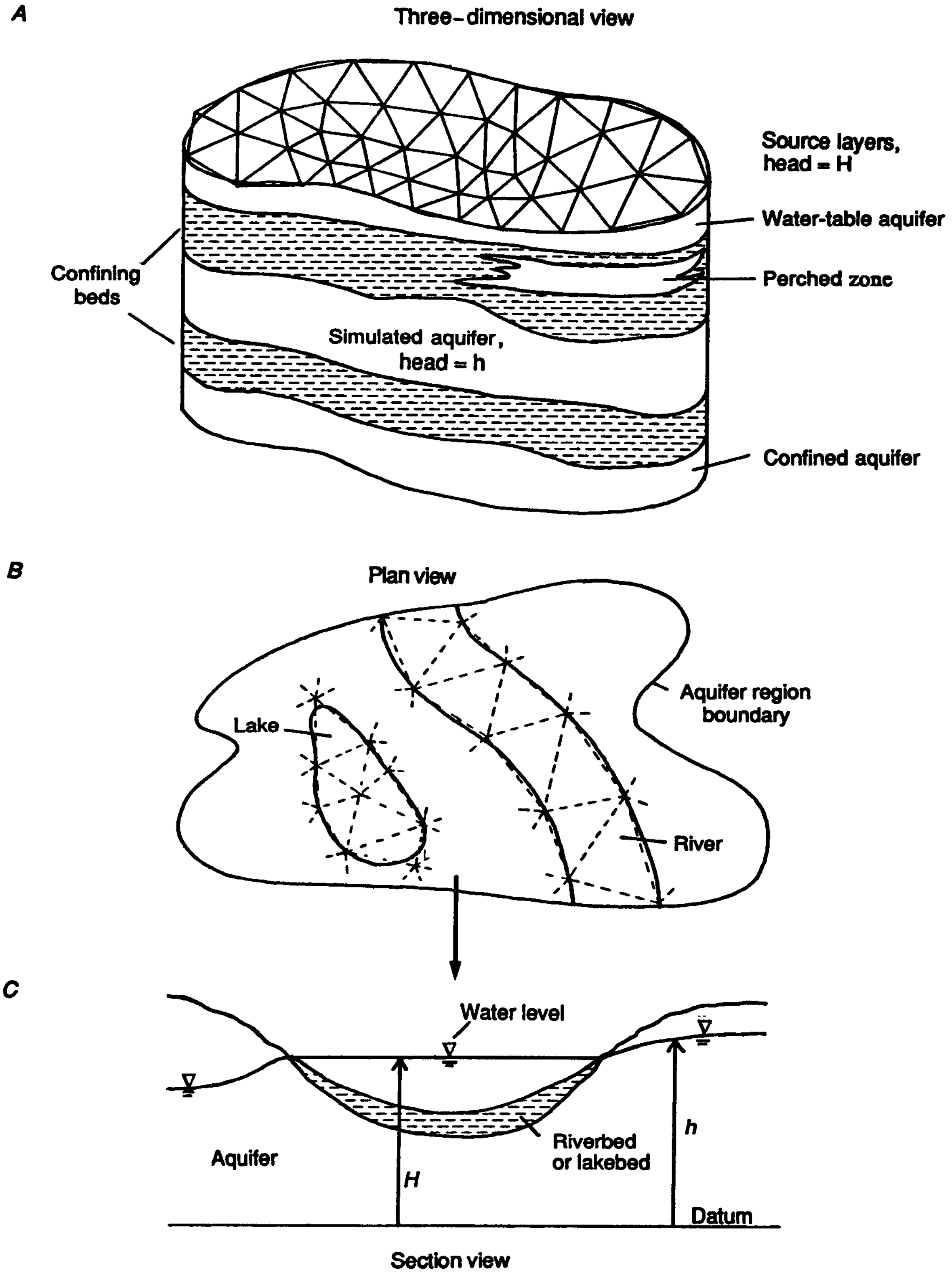


Figure 10.—Examples of steady vertical leakage (*A*) from source layers and (*B*) and (*C*) from areally extensive surface-water features.

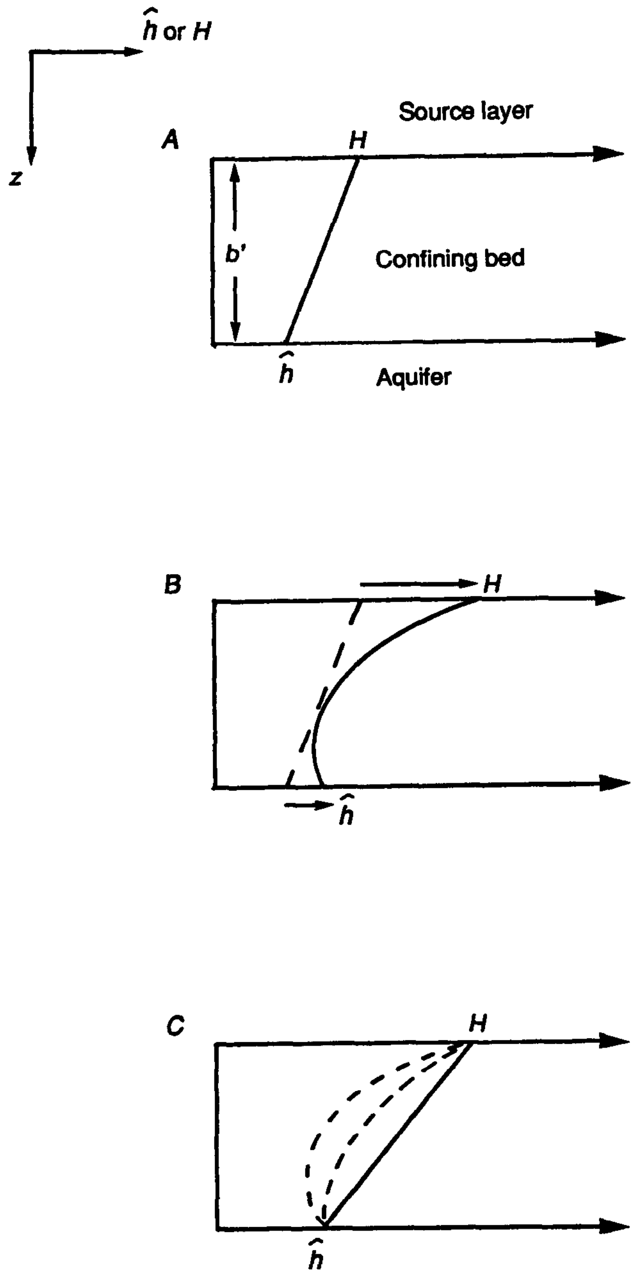


Figure 11.—Vertical head distributions in a confining bed for (*A*) initial, steady-leakage conditions at time $t=t_n$; (*B*) transient conditions following changes to aquifer head, $\hat{h}$, and source-layer head, H, at $t=t_n+\Delta t_{n+1}$; and (*C*) re-establishment of steady-leakage conditions at $t>>t_n+\Delta t_{n+1}$.

pate within the confining bed in response to head changes at the confining-bed boundaries (fig. 11*A*,*B*). These head changes commonly are the result of changing stresses in the aquifer, such as changing or initiating well pumpage, or changing fluxes or controlling heads to aquifer-boundary conditions. If the conditions causing the head changes at the confining-bed boundaries are fixed in time, then the nonsteady hydraulic gradients will adjust gradually until a new steady-state condition is established (fig. 11*C*). Depending on the direction of head changes at the boundaries of the confining bed, water is either released from or taken up by storage in the confining bed. This process creates nonsteady (transient) leakage rates across the boundaries of the confining bed that differ substantially from those that are calculated if yield from storage effects in the confining bed is neglected (steady leakage).

The existence and magnitude of transient-leakage effects on the flow system is related to the physical and hydraulic properties of the confining bed, the magnitude of head changes at its vertical boundaries, and the relative time over which the aquifer head is simulated. Transient-leakage effects are not present during steady-state simulations because steady-state ground-water flow is independent of time, whereas transient effects are time dependent. For nonsteady-state conditions in the aquifer, flow rates from transient leakage can vary within orders of magnitude either at a given location during the simulation period or throughout the model area at a given instant in time.

The importance of transient-leakage effects on the vertical leakage rate can be determined by evaluating a term called dimensionless time. Dimensionless time is expressed in the equation development of Cooley (1992) as the product of simulation time and the confining-bed properties of thickness, vertical hydraulic conductivity, and specific storage. The confining-bed properties are given as γ_i in equation (167) in Cooley (1992), and time is either the total simulation time or the time-step size. Dimensionless time is used in the expressions for approximating transient-leakage flux during a time step. In general, these expressions contain two infinite series that are approximated with exponential functions over dimensionless time to obtain the transient-leakage flux (see development leading to equation (198) in Cooley, 1992). The series and the approximating functions indicate that transient-leakage effects are an important part of the leakage rate when dimensionless time is less than about 0.1. For values of dimensionless time greater than about 0.1, the transient-leakage effects can be neglected, as contributions to the leakage rate from the series and the exponential functions are small, and the leakage rates can be approximated by steady vertical leakage (discussed in the previous section).

The formulation for γ_i in equation (167), (Cooley, 1992), and the simulation time can be used to evaluate the effects of transient leakage on the vertical leakage rate. The term γ_i indicates that, for a given simulation time, transient-leakage effects will be present and persist during the simulation (values of dimensionless time less than 0.1) if the confining bed is thick and has a low vertical hydraulic conductivity than if it is thin and has a higher vertical hydraulic conductivity. Similarly, for a given set of confining-bed properties, transient-leakage will have more of an affect on the computed hydraulic head for simulations of short duration than for simulations of long duration. The user can determine the importance of transient leakage on the vertical leakage rate by computing γ_i for each zone that contains a different set of confining-bed properties, and multiplying the γ_i values by simulation time to compute dimensionless time.

Transient-leakage effects usually are larger than steady-leakage effects during the time immediately following changes to stresses or boundary conditions, as nonsteady vertical gradients are at their maximum at this time. The transient effects gradually diminish with time as stresses and boundary conditions remain constant during the simulation, leaving only steady leakage to characterize the flow rate across the confining bed. However, it is possible for nonsteady vertical hydraulic gradients to persist throughout the simulation period, making transient-leakage effects an important water-budget component for the aquifer.

The transient-leakage approximation in MODFE is a linear process that is applied to nonsteady confined- and unconfined-flow problems. It may be required, however, when simulating other (nonlinear) features in combination with transient leakage, as shown in the structures of the main program in the section "Program Structures and Lists of Main Programs," (Torak, 1993).

Inputs for transient leakage consist of the vertical hydraulic conductivity and specific storage of the confining bed. Also, the inputs of vertical hydraulic conductance (VLC) and the source-layer head (HR), which were described in the section "Steady Vertical Leakage", are required for simulating transient leakage. The values for VLC and HR are used in computations for steady and transient leakage, and are input once for both formulations. The vertical hydraulic conductivity and specific storage are represented in MODFE as the program variables VCON and SPST, respectively, and are input by hydraulic-property zone. Details of preparing data for input by hydraulic-property zone are given in the section "Hydraulic-Property and Boundary-Condition Zones."

Areally Distributed Sources and Sinks

Areally distributed stresses, such as precipitation, infiltration from applied recharge, or a constant evapotranspiration rate, can be simulated by MODFE. These stresses are represented in equation (1) and in figure 12 as the term W, which is the unit areal recharge or discharge rate (volumetric flow rate per unit area). W has dimensions of [length/time].

Values for the unit rate are represented in MODFE as the program variable QD, and are input by hydraulic-property zone. Within MODFE, the unit rate is multiplied by one third of the element area, $(1/3)\Delta^e$ (fig. 12), so the volumetric flow rate for the areally distributed stress can be applied to each node in the element. Details of these computations are given in the section "Areally Distributed Sources and Sinks" in Torak (1993).

The unit rate of areally distributed stress is allowed to vary with time in MODFE. New unit rates can be input for a time step or a stress period. Details of changing areally distributed stresses with time are given in the sections "Input Instructions" and "Changing Stresses and Boundary Conditions with Time" (Torak, 1993).

Point Sources and Sinks

Point sources and sinks, such as wells and constant-flow drains, can be simulated by using MODFE. These features are represented in equation (1) as the term P. A specified-flow condition also can be simulated as a point source or sink; however, it usually is represented by the specified-flow part of a Cauchy-type boundary, which is described in the section "Boundary Conditions."

Point sources and sinks are represented in MODFE by assuming the stress is located at a node. Thus, nodes are positioned at locations of the stress or anticipated stress when the mesh is designed. The flexibility in mesh design allows nodes to be placed at the location of the point stress for most problems.

If nodes cannot be positioned at the location of the point stress within the model region, then the point stress can be distributed to the nodes of the element in which the stress is contained by assuming linear variation of the stress within an element. The point stress is apportioned to the nodes of an element in the same manner as hydraulic head at any location within an element is defined by the head at the nodes (see equation (8) in Cooley, 1992). Values for the coordinate functions, N_i, given by equations (9)–(11) in Cooley (1992), are used to weight the point stress proportionately at the three nodes. These values can

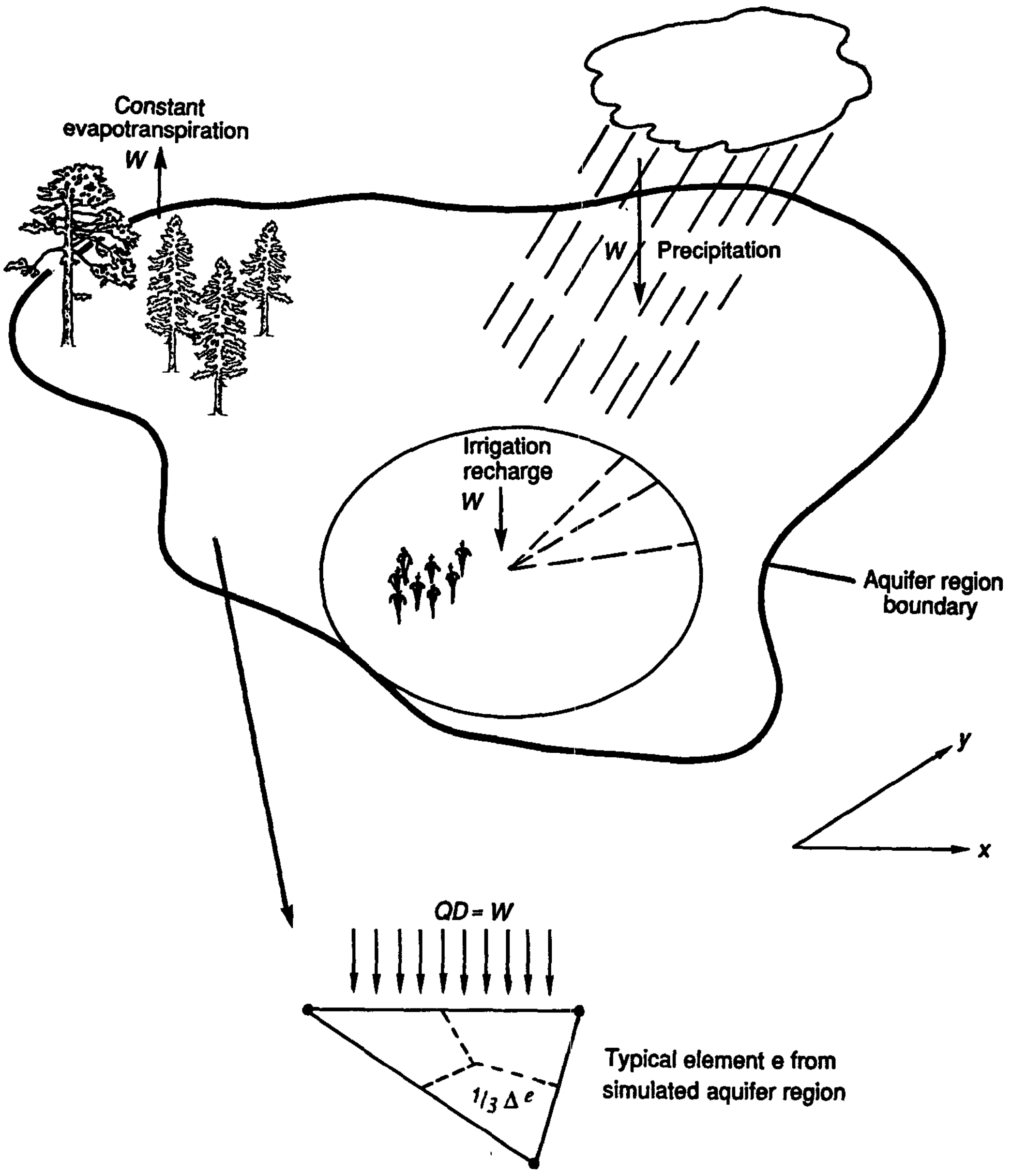


Figure 12.—Areally distributed stress on aquifer region and representation by a typical element.

be obtained by hand calculations or from a small computer program by utilizing the x-y coordinates of the point stress and of the nodes defining the element. However, care should be taken in applying this technique to relatively small elements so that the geometry of the aquifer problem is preserved.

Data inputs for point sources and sinks consist of the node number where the stress is located and the volumetric flow rate. The volumetric flow rate is represented in MODFE as the program variable QWEL, and the node number is represented as the program variable J. Prior to these inputs, the number of point sources and sinks that are simulated initially is input as the program variable NWELS.

The values and locations of point stresses can be changed before any time step or stress period of the simulation. Details of the data inputs required for changing point stresses with time are given in the section “Changing Stresses and Boundary Conditions with Time.” Instructions for establishing stress periods and time-step sizes are given in the section “Selecting Stress-Period and Time-Step Sizes.”

Initial Condition of Hydraulic Head

Equation (1) is subject to the initial condition of hydraulic head given by equation (5) in Cooley (1992), or

$$h(x,y,t) = h_o(x,y), \qquad (2)$$

where $h_o(x,y)$ is the head or reference altitude at a node located at a point (x,y) in the aquifer at the start of the simulation period (at t=0). Values for $h_o(x,y)$ can be the altitude of the potentiometric surface, the water-table, or some other value to which the computed heads are referenced. For axisymmetric coordinates, $h_o(x,y)$ is replaced by $h_o(r,z)$ in equation (2). Head is represented in MODFE by the program variable H. The initial values of hydraulic head are input at each node. In subsequent computations, H represents different values before it becomes the computed solution. For simulation of transient conditions, H represents first the average hydraulic head during the time step, and then the head at the end of the time step. This latter value is used as the initial condition of head for the next time step or as the computed solution. For steady-state simulations, H represents either the head at the end of the current iteration or the initial condition at the beginning of the next iteration.

Boundary Conditions

MODFE can simulate three types of boundary conditions to equation (1): specified head (Dirichlet), specified flux (Neumann) and mixed (Cauchy). Each type is represented by equation (4) of Cooley (1992). The specified-flux and specified-head conditions are special cases of the mixed condition (see Bear, 1979, p. 117–120 for a description of these boundary conditions). Computations for the specified-flux and mixed conditions are combined in MODFE; the specified-head condition is formulated separately from the other two conditions. Because of the relation between specified-flux and mixed conditions, they are referred to as Cauchy-type boundaries in this documentation. Examples showing the application of specified-head and Cauchy-type boundaries to aquifer problems and their implementation in MODFE are given in the following sections. The Cauchy-type condition is separated into two components; specified flux and head-dependent flux. Each component is discussed separately as they have different hydrologic applications to ground-water flow.

Specified Head

The specified-head, or Dirichlet, condition is one in which hydraulic head is known at an aquifer boundary and is fixed during the simulation. Specified-head boundaries occur when the aquifer region is in direct hydraulic connection with a body of water whose level is either constant or varies in a predictable manner over time and is not affected by stresses in the aquifer. A specified-head condition also can exist along the boundary of the model region (but not necessarily the aquifer boundary) where the hydraulic head is known and is unaffected by stresses within the aquifer.

Examples of specified-head boundaries are shown in figure 13. These are: (1) a river or (2) a lake, both fully penetrating the aquifer and having a known water level, (3) an ocean-discharge boundary where the freshwater head at the shore is known, and (4) the boundary of the simulated region, where the head along the boundary is known and is not expected to vary in response to stresses in the aquifer. Although specified-head boundaries are suitable for representing the hydrologic features shown in figure 13, other boundary conditions, discussed in later sections, may be more appropriate for simulating these features than the specified-head condition.

Specified-head boundaries are represented in MODFE by assigning boundary heads to nodes. Values for specified-head nodes are input as the program variable HB (fig. 13). Prior to the input of HB, the number of nodes used to simulate specified-head conditions is input as the program variable NHDS. For steady-state simulations, at least one specified-head condition (node) is required in order to obtain a unique solution to the aquifer problem. (This mathematical requirement also can be satisfied by at least one head-dependent, Cauchy-type boundary, described in a following section.)

Head values on specified-head boundaries can be constant for the entire simulation period, or they can vary as functions of time. Descriptions of the data inputs and the program structure required to change boundary conditions with time are given in the section "Changing Stresses and Boundary Conditions with Time," and in the section "Changing Stresses and Boundary Conditions with Time" in Torak (1993).

Specified Flux

A specified-flux, or Neumann, condition is one in which the normal component of ground-water flow is known across a boundary. This is a special case of the mixed (Cauchy) condition, and is obtained from equation (4) in Cooley (1992) by setting $\alpha = 0$. The specified-flux condition is defined in equation (4) as the term q_B [length^2/time], which represents a unit discharge rate across the boundary, or volumetric flow rate per unit length of boundary (fig. 14). It is used where the volumetric flow rate, $Q_B = q_BL$, is pre-

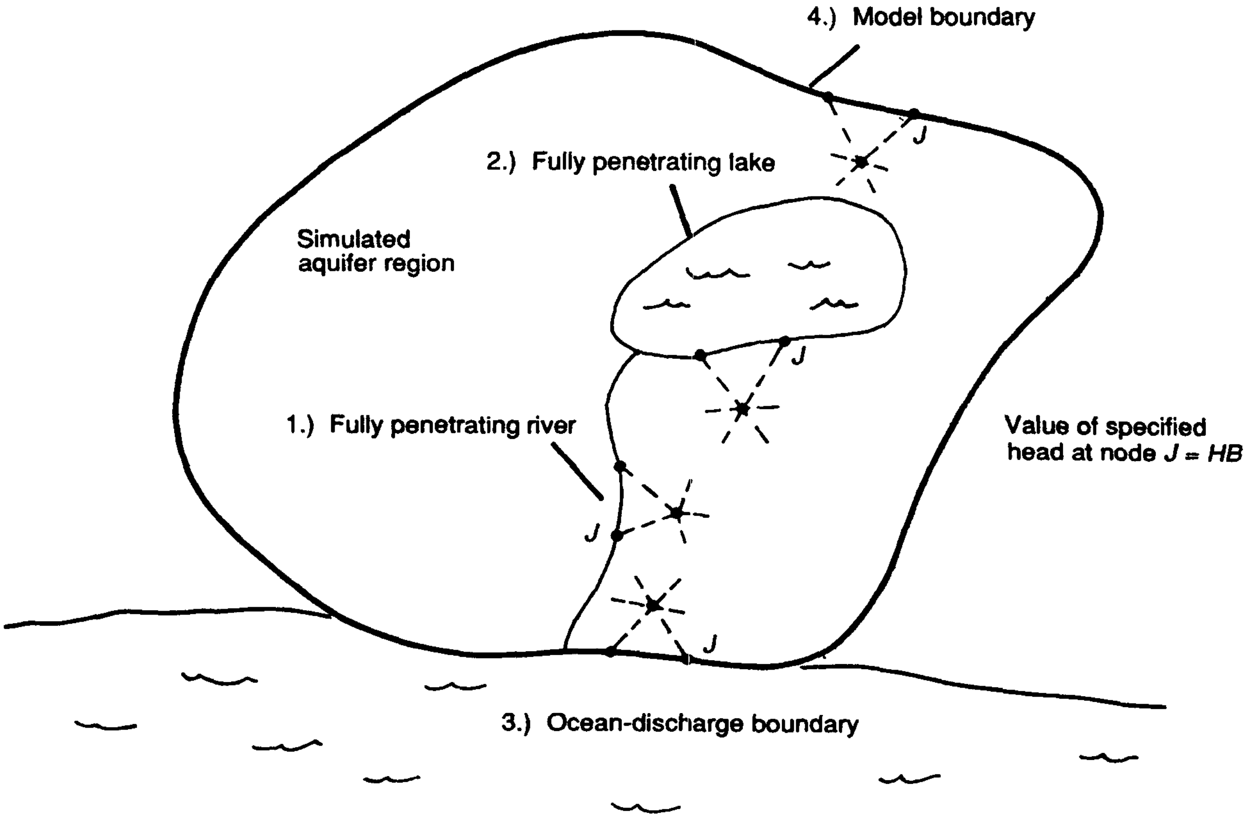


Figure 13.—Applications of specified-head boundaries for a simulated aquifer region and nomenclature used in MODular Finite-Element model (MODFE).

scribed across internal or external boundaries of the model region during simulation, where L is the length of the boundary.

Examples of specified-flux boundaries are regional flow across an external model boundary, constant-flow drains, and flow to a well in cross section (fig. 14). Specified fluxes from regional flow usually result from selecting a model area that is smaller than the areal extent of the aquifer. For this case, the specified-flux condition accounts for flow rates across model boundaries that emanate either from outside the model area or from within the model area and are not expected to change during the simulation. Other examples of specified-flux boundaries in aquifer cross sections or in axisymmetric (radial) problems are given in the sections "Cross Sections" and "Axisymmetric Flow." A special case of a specified-flux condition is a zero-flux, or impermeable, boundary.

The manner in which the unit discharge rate q_B is obtained for input to MODFE varies with each application of the specified-flux condition. For most applications (fig. 14*A*,*B*), q_B is obtained by dividing the volumetric flow rate Q_B by L, the length of the boundary along which Q_B is known. However, as discussed below, q_B requires other computations in order to represent the effects of areally distributed recharge over the region outside the simulated model area. Zero-flux or impermeable boundaries do not require specification of q_B as they are represented automatically along external boundaries of the model area.

The computation of the unit discharge rate q_B to represent areally distributed recharge located outside the model area depends on the geometry of the model boundary (fig. 14*C*). For curved model boundaries, q_B can be approximated by flow within a converging stream tube, whereas for relatively straight boundaries, q_B can be approximated by flow within a parallel stream tube. For a parallel stream tube, the unit discharge is computed as $WL_s/2$, where W is the unit rate of areally distributed recharge (or discharge), from equation (1), and L_s is the distance from the model boundary over which W is applied. For a converging stream tube, q_B is given by

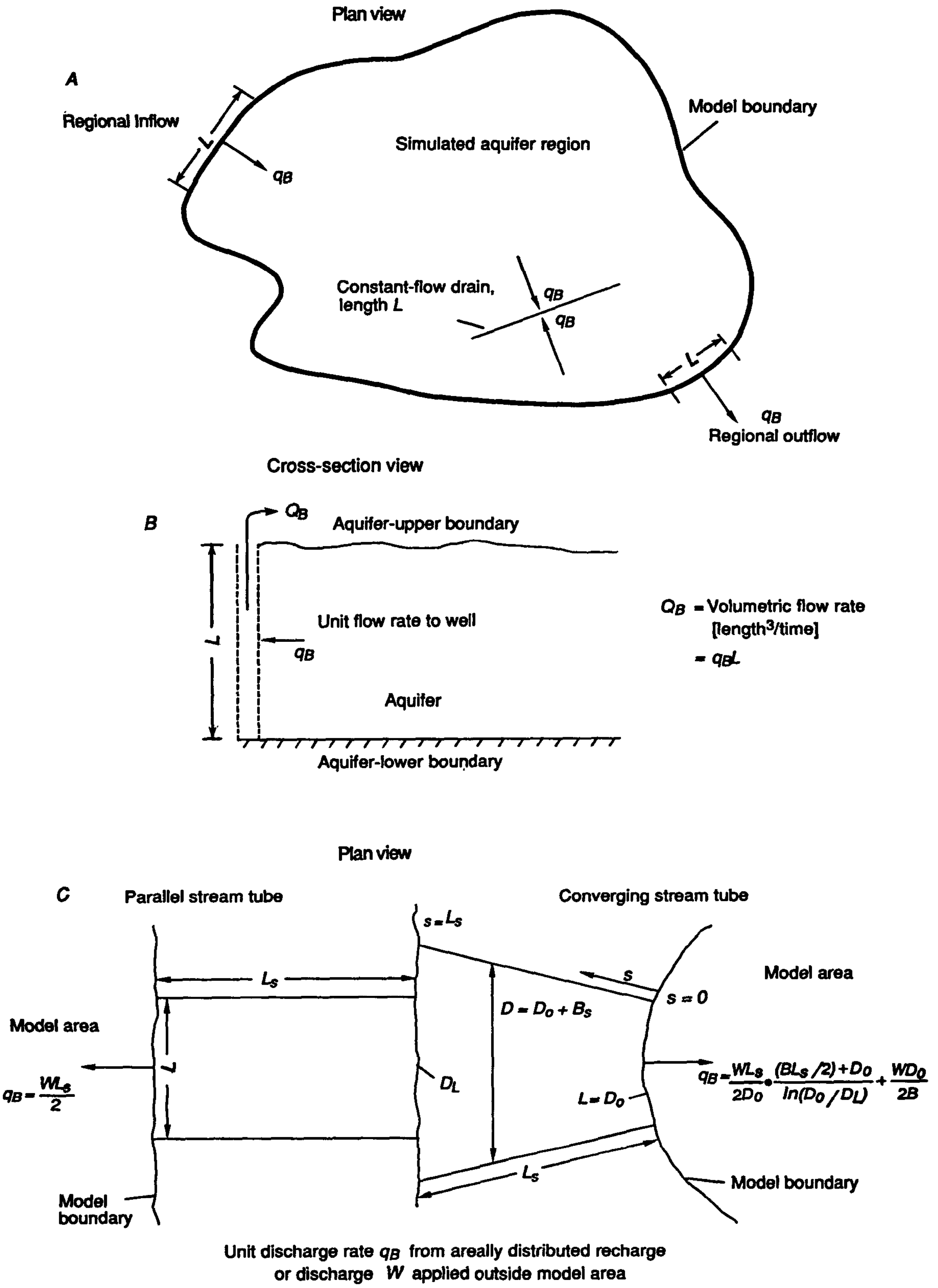


Figure 14.—Specified-flux boundaries representing (*A*) regional inflow and outflow and internal drainage; (*B*) constant flow to a well in cross section; and (*C*) areally distributed recharge or discharge outside simulated aquifer region.

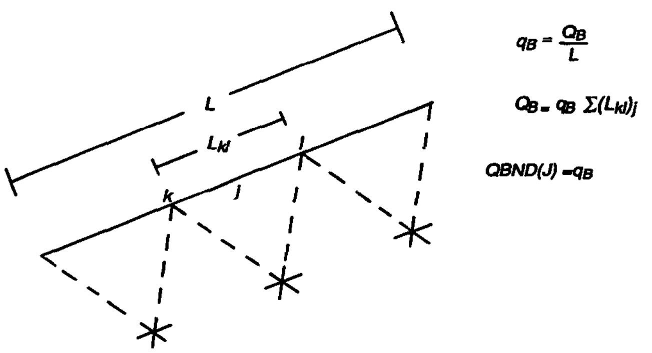


Figure 15.—Specified-flux boundary having length *L* and volumetric flow rate Q_B, subdivided by element sides *j*, and nomenclature used in MODular Finite-Element model (MODFE).

$$q_b = \frac{WL_s}{2D_o} \times \frac{\left(\frac{BL_s}{2}\right) + D_o}{\ln\left(\frac{D_o}{D_L}\right)} + \frac{WD_o}{2B} \qquad (3)$$

where D_o and D_L are the widths of the stream tube at the model boundary and at the distance L_s from the boundary, respectively. The value of q_B accounts for an increased width, D, of the stream tube with distance, s, from the boundary. The rate at which D increases with s is given by B and is incorporated into the computation of q_B.

Specified-flux boundaries are represented in MODFE by element sides (fig. 15). Values for the unit discharge rate q_B are input to MODFE by boundary side j as the program variable QBND(J). Node numbers k and l defining element side j are input with QBND(J), respectively, as the program variables KQB(J) and LQB(J). Boundaries that use more than one element side to represent the total length L require separate input of QBND(J) for each side. Element sides containing the same values of QBND(J) can be grouped into boundary-condition zones to facilitate data input (see section "Hydraulic-Property and Boundary-Condition Zones").

The number of specified-flux boundaries (element sides) is summed with the number of head-dependent boundaries and is input to MODFE as the program variable NQBND. The value of NQBND is used to dimension storage locations and to control computations in MODFE that involve Cauchy-type boundaries. Programming details for these boundary conditions are given in the section "Specified-Flux Boundaries" in Torak (1993).

The unit discharge rate on specified-flux boundaries can vary as a function of time or be constant during the simulation period. Details on changing boundary conditions with time are given in the section "Hydraulic-Property and Boundary-Condition Zones."

Head-Dependent (Cauchy-Type) Flux

The head-dependent (Cauchy-type) condition relates the normal component of ground-water flow across a boundary to a head difference. The boundary condition is given by equation (4) of Cooley (1992) with $q_B = 0$. The head-dependent (Cauchy-type) flux yields steady-flow rates (no storage effects) across the boundary, in that the head difference, $H_B - h$ is related to the flow rate by a scalar function, α. The meaning of α varies depending on the application of the flux condition. However, α should not be set to a large value to create the specified-head (Dirichlet) condition as this condition is formulated differently in MODFE (see previous section). Because of this limitation on α, the true, mixed (Cauchy) condition is not represented in MODFE; instead, a Cauchy-type condition is formulated.

The head-dependent (Cauchy-type) flux has many applications to simulating ground-water flow (figs. 16–18). This boundary condition usually is needed when the model area is smaller than the physical extent of the aquifer, and regional flow occurs across model boundaries. Similarly, the head-dependent (Cauchy-type) flux allows ground water to flow across model boundaries in response to stresses, such as wells, that are operating near the boundaries within the model area. Aquifer drawdown is permitted at model boundaries by using this boundary condition. However, because the flow rate across the boundary is steady, the effects of storage or stresses outside the model area are not represented by the head-dependent (Cauchy-type) flux. Thus, model boundaries should be established so that only small percentages of the total drawdown from a well reach the boundary. (The specified-flux condition can be used to represent areally distributed stresses in the region outside the model area, as discussed in the previous section.)

Within the model region, head-dependent (Cauchy-type) fluxes can represent leakage to or from rivers, drainage ditches, fracture or fault zones, or other line-oriented features. In cross sections or in axisymmetric flow, head-dependent-flux conditions can represent lateral or vertical flows across model boundaries, such as regional flow, vertical leakage, or flow along fracture or fault zones. Applications of head-dependent (Cauchy-type) flux to cross-section and axisymmetric problems are described, respectively, in the sections "Cross Sections" and "Axisymmetric Flow."

Head-dependent (Cauchy-type) boundaries are represented in MODFE by element sides (figs. 16*B*, 17*B*,*C*, and 18). Values for α are required for each element side j on a boundary, and external heads H_B are defined for boundary nodes k and l. The term α is represented in MODFE by program variable ALPH(J). Nodes k and l defining element side j are represented, respectively, as the program variables KQB(J) and LQB(J). External or boundary heads H_B are represented as the program variables HK(J) and HL(J) for nodes k and l, respectively. Boundary sides that contain the same α value can be grouped into zones to facilitate data input. Details of establishing boundary-condition zones are given in the section "Hydraulic-Property and Boundary-Condition Zones."

The computation of α for simulating regional flow across model boundaries as head-dependent (Cauchy-type) fluxes is dependent on boundary geometry. Flow across highly curved model boundaries is approximated by a converging stream tube, and flow across relatively straight boundaries is approximated by a parallel stream tube (fig. 16*A*). For a parallel stream tube, the α value is computed as T/L_c, where T is the average transmissivity of the aquifer (or other porous material) between the model boundary and H_B, and L_c is the distance from the boundary to H_B. For a converging stream tube, α is computed as $TB/[D_o \times \ln(D_o/D_L)]$, where T is transmissivity as defined above, and D_o and D_L are the widths of the stream tube at the model boundary and at the distance L_c from the boundary, respectively. The value of α for a converging stream tube accounts for the increase in width, D, of the stream tube with distance, s, from the boundary. The rate of increase of D with s is given by B and is incorporated into the computation of α for the converging stream tube.

For simulating regional flow as a head-dependent (Cauchy-type) boundary, the external head H_B is located sufficiently far from the model boundary so that head changes at the boundary are not transmitted to H_B (fig. 16). Head changes over L_c are assumed to be linear; that is, steady hydraulic gradients are assumed to exist in the region between the model boundary and H_B.

To simulate leakage to or from a river, drainage ditch, or other line-oriented, leaky, surface-water feature (fig. 17), α is computed as the product of the vertical hydraulic conductance (vertical hydraulic conductivity divided by thickness) of the surface-water sediments and the width of the feature. The boundary head H_B is the surface-water level, such as river stage. These properties of the boundary condition are shown in figure 17*A*, where W_r is width and b_r is thickness. The term α is given by $(K_rW_r)/b_r$, where K_r is vertical hydraulic conductivity. In computations within MODFE, α is multiplied by the length of element side j on the boundary, L_{kl}, to give the area across which flow occurs.

The head-dependent (Cauchy-type) condition can be used to represent ground-water flow across a fault or fracture zone. The flow is analogous to steady vertical leakage except that it occurs along element sides, which are aligned with the trace of the fault or fracture zone in the aquifer (fig. 18), instead of occurring over the area of elements as in vertical leakage. The α term contains hydraulic properties that characterize the material within the fault or fracture zone. These properties are the vertical hydraulic conductivity, K', width, W', and thickness, b', of the fault or fracture zone. An element side can be bounded from above, from below, or from above and below, by the head-dependent (Cauchy-type) condition. The boundary head H_B is the source-layer head or other head external to the aquifer that is associated with providing a boundary flow along the fault or fracture zone.

Values for the boundary or external head H_B can be changed as a function of time during the simulation. Details of this procedure are given in the section "Changing Stresses and Boundary Conditions with Time."

Cross Sections

MODFE can be used to simulate ground-water flow along a cross section defined by a stream line. Cross sections usually are constructed to determine horizontal and vertical components of ground-water flow that are associated with stresses, boundary conditions, and other hydrologic features. Typical applications of cross sections are to simulate the head distribution in the vicinity of a fully or partially penetrating river, infiltration gallery, or similar set of line-oriented stresses (wells) (fig. 19), and to determine the effects of vertical leakage on a system of aquifers and confining beds (fig. 20*A*). Cross-section simulations can be performed on a confined aquifer or on a system of confined aquifers and confining beds in steady or nonsteady state. Because MODFE does not contain the formulation of a moving boundary for the phreatic surface, only steady-state conditions can be simulated for an unconfined aquifer. (For cross sections of unconfined aquifers in steady state, the phreatic surface is a no-flow or specified-head boundary.)

Inputs and program variables in MODFE take on different meanings for cross-section simulations than for simulations in the areal plane. For cross sections, hydraulic conductivity is input for one horizontal direction (x or y) and for the vertical direction as the program variables XTR and YTR, respectively.

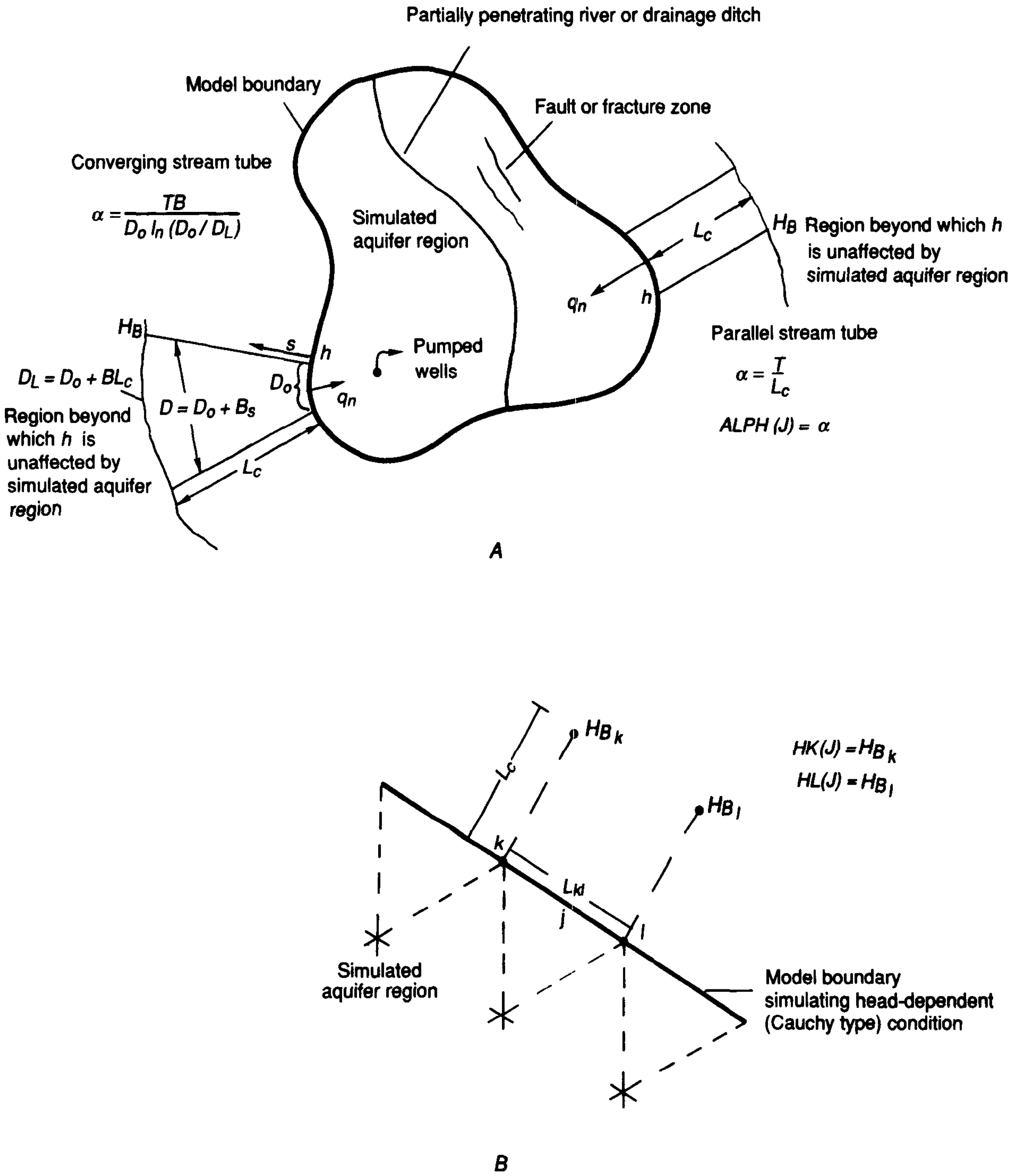


Figure 16.—(*A*) Examples of head-dependent (Cauchy-type) flux q_n across simulated aquifer boundaries; and (*B*) subdivision of boundary using element sides and nomenclature used in MODular Finite-Element model (MODFE).

These program variables usually represent aquifer transmissivity in the x and y directions, respectively, for areal simulations. Specific storage [length^{-1}] is input as the program variable STR for cross sections instead of the aquifer storage coefficient [dimensionless] for areal simulations.

Because the finite-element mesh is oriented in the vertical plane, boundary conditions and stresses that

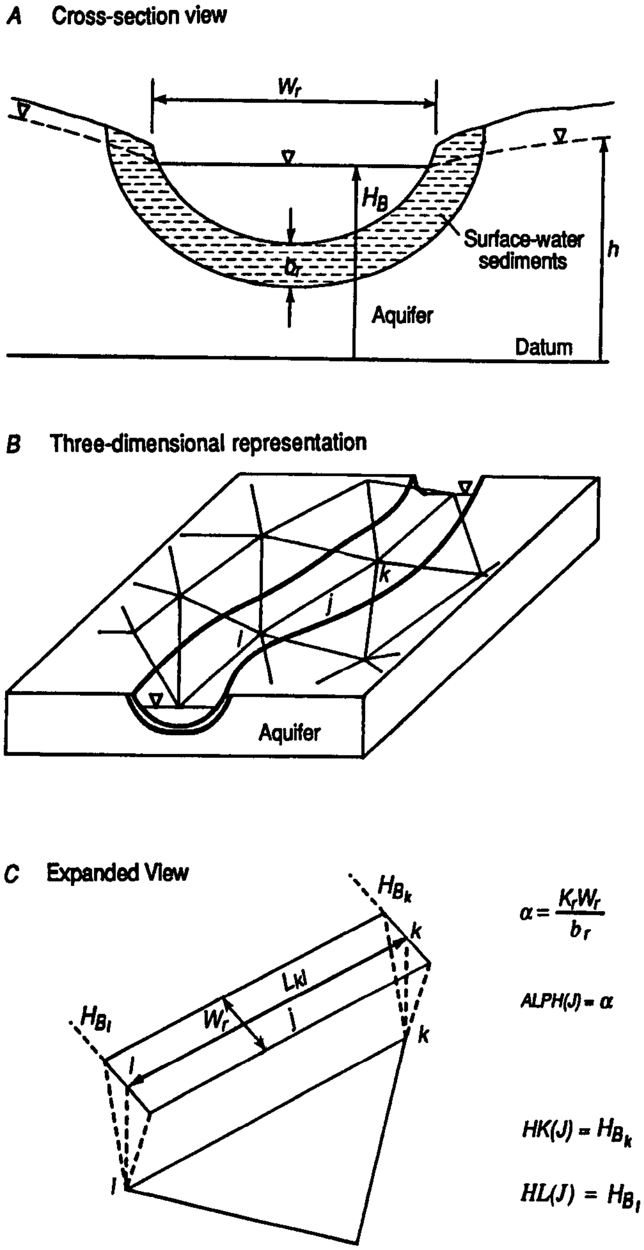


Figure 17.—Rivers represented as head-dependent (Cauchy-type) boundaries; (*A*) cross-section view of river and aquifer; (*B*) three-dimensional representaion of river and aquifer, partially subdivided with finite elements; and (*C*) plan view of element on boundary and nomenclature used in MODular Finite-Element model (MODFE).

are applied to aquifer problems in the areal directions are represented differently in cross section. Stresses and boundary conditions that are represented by points or lines in the areal plane are extended vertically in the cross section and become, respectively, line or areal stresses and boundary conditions (fig. 19). Areal hydrologic features such as vertical leakage and areally distributed recharge are represented as line features in cross-section simulations (fig. 20*A*,*B*). Regional flow across model boundaries is represented as flow across element sides in a manner similar to the representation of regional flow in the areal plane, except the element side is oriented vertically in the plane of the cross section instead of horizontally (fig. 20*C*). In cross section, these hydrologic features are represented as Cauchy-type boundaries, either as specified-flux or as head-dependent (Cauchy-type) flux conditions.

Applications of Cauchy-type boundaries for cross-section simulations are described here using terms that were defined in the sections "Specified Flux" and "Head-Dependent (Cauchy-Type) Flux." The user is referred to those sections for details about Cauchy-type boundaries.

A unit thickness ($b=1$) is assumed to exist normal to the plane of the cross section (figs. 19 and 20). This value is used to complete the formulation of flow across an element side by providing an area across which boundary fluxes and stresses can occur. The unit thickness is included in the following discussions, although it is excluded from computations in MODFE.

Ground-water flow to a fully or partially penetrating river can be simulated in cross section by using the head-dependent (Cauchy-type) condition (fig. 19*A*). The boundary flow is controlled by the head difference ($H_B - h$) and the hydraulic properties of the riverbed sediments. The α term is given as $K_r b/b_r$, where K_r and b_r are the hydraulic conductivity and thickness, respectively, of the riverbed sediments, and b is the unit thickness of the cross section. The river stage is represented as the boundary or external head H_B.

Constant flow to a line of wells or from an infiltration gallery can be represented in cross section by using the specified-flux condition (fig. 19*B*). The volumetric discharge (or recharge) rate, Q_B, is divided by the length of the screened interval or open hole in contact with the aquifer, L, and the distance between wells, L_w, to obtain a unit discharge, q_B, for the specified-flux condition. The unit discharge represents the volumetric flow rate per unit thickness of the cross section, per unit length of screened interval or open hole. For multiple aquifers or for nonhomogeneous conditions, Q_B is proportioned according to the flow rate, q_{Bi}, and length, L_{zi}, of each zone i that contributes or receives water across the boundary (fig. 21). Thus, different discharge or recharge rates can be represented by boundary-condition zones having different values of q_{Bi}. The sum of the flow rates q_{Bi} over all boundary-condition zones gives the value Q_B/L for the multiaquifer or nonhomogeneous system.

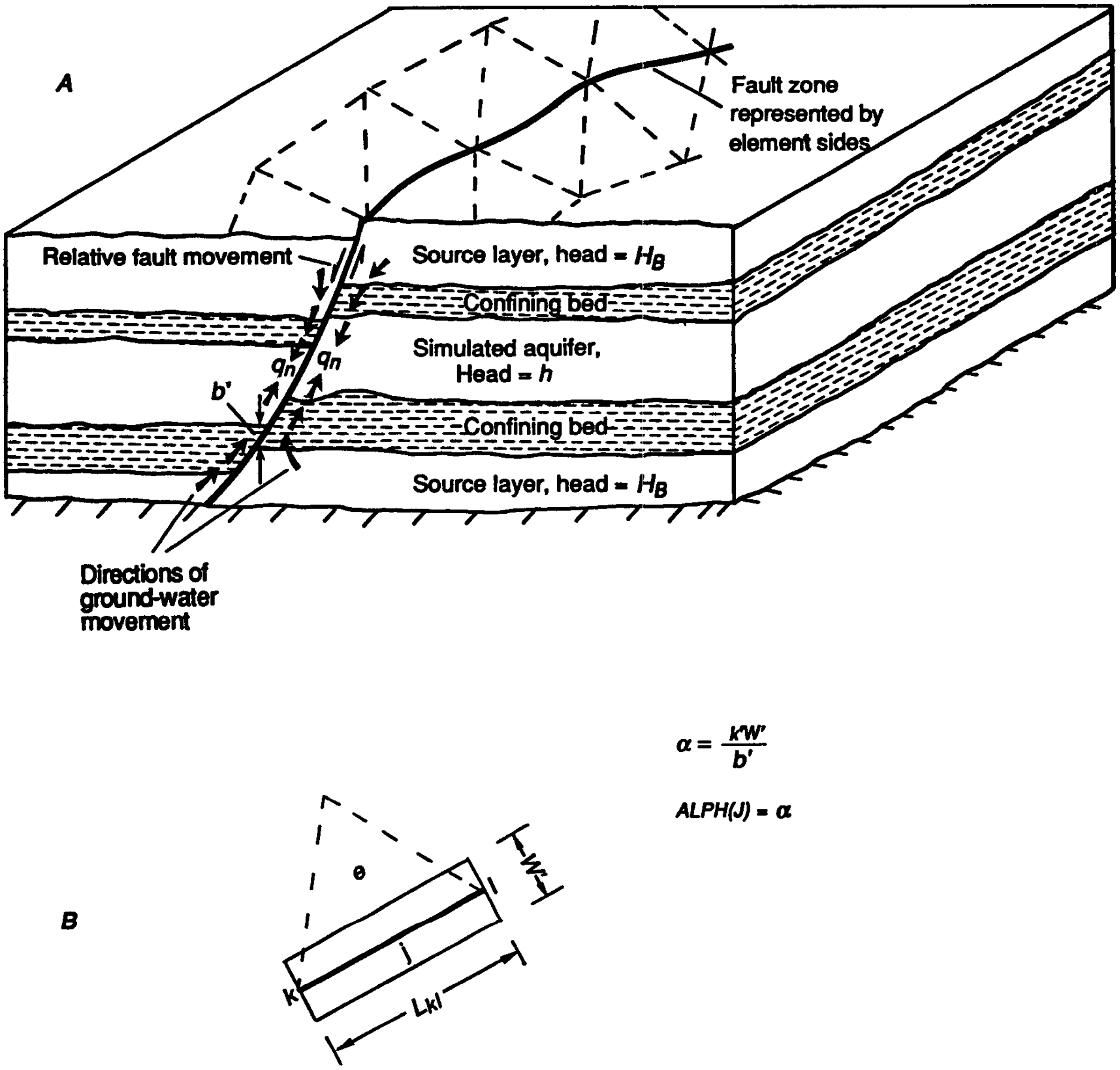


Figure 18.—Ground-water flow along fault zone represented as head-dependent (Cauchy-type) boundaries; (*A*) three-dimensional representation of simulated aquifer, partially subdivided with finite elements with ground-water flow along fault zone; and (*B*) plan view of element side on boundary.

Steady-vertical leakage is simulated in cross section as a head-dependent (Cauchy-type) boundary (fig. 20*A*). The external or boundary head H_B for this application of the boundary condition represents the source-layer head. The α term is computed as the product of vertical hydraulic conductance (vertical hydraulic conductivity divided by thickness) and unit thickness normal to the plane of the cross section. This computation is given as $K'b/L_c$ in figure 20*A*, where K′ is the vertical hydraulic conductivity of the material between the aquifer and the source-layer head, H_B, b is the unit thickness of the cross section, and L_c is the distance from the boundary to the source-layer head H_B. Usually, K′ is the vertical hydraulic conductivity of a confining bed and L_c is confining-bed thickness.

Regional flow across model boundaries is represented in cross-section by head-dependent (Cauchy-type) flux conditions (fig. 20*C*). The α term is computed as Kb/L_c, where K is the horizontal hydraulic conductivity (either the x or y direction in the plane of the cross section) of the material in the region between boundary side j and the external head H_B; b is the unit thickness of the cross section, and L_c is the distance from side j to H_B.

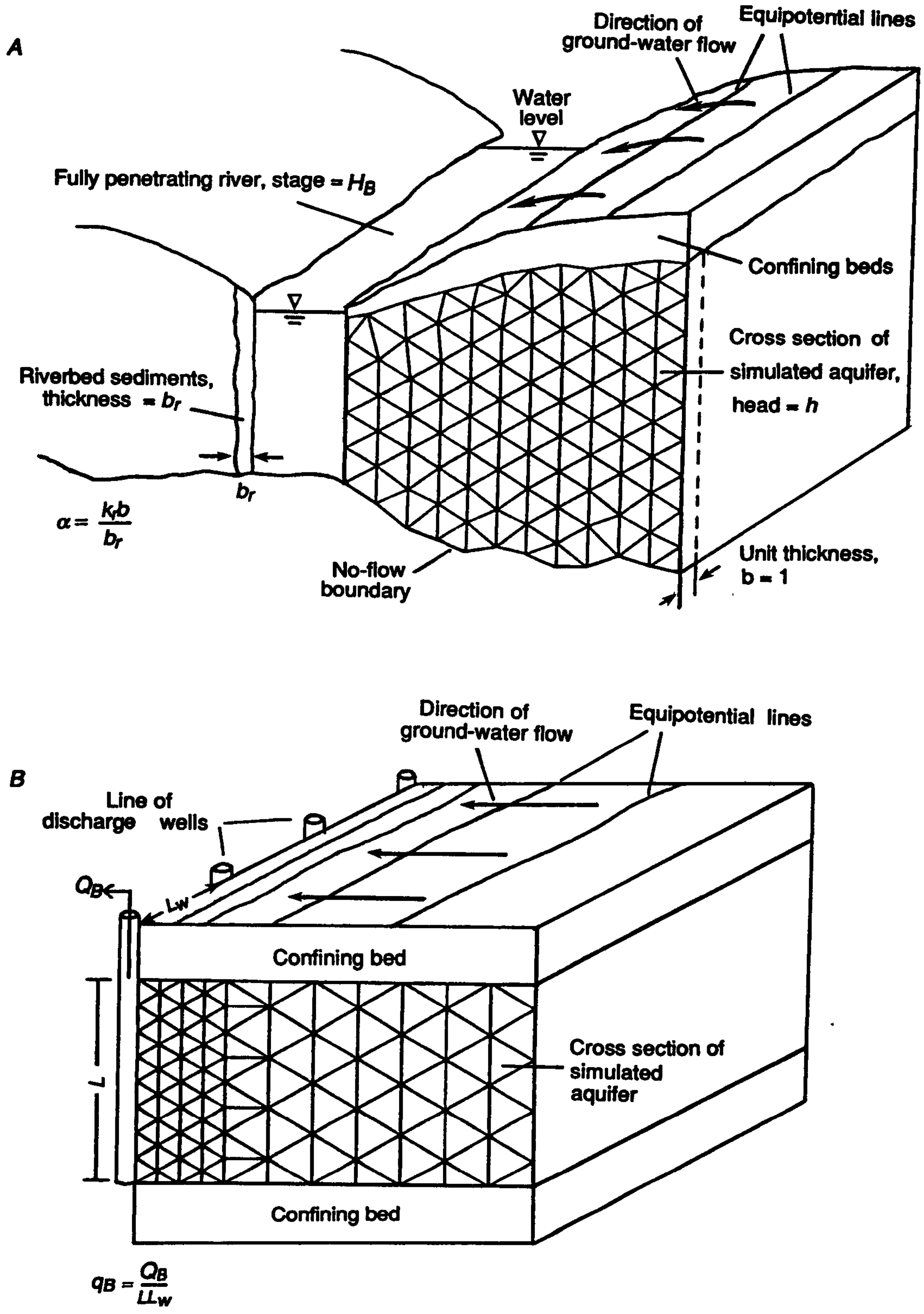


Figure 19.—Cauchy-type boundaries used in cross section to represent (*A*) fully penetrating river; and (*B*) line of discharge wells having volumetric flow rate Q_B.

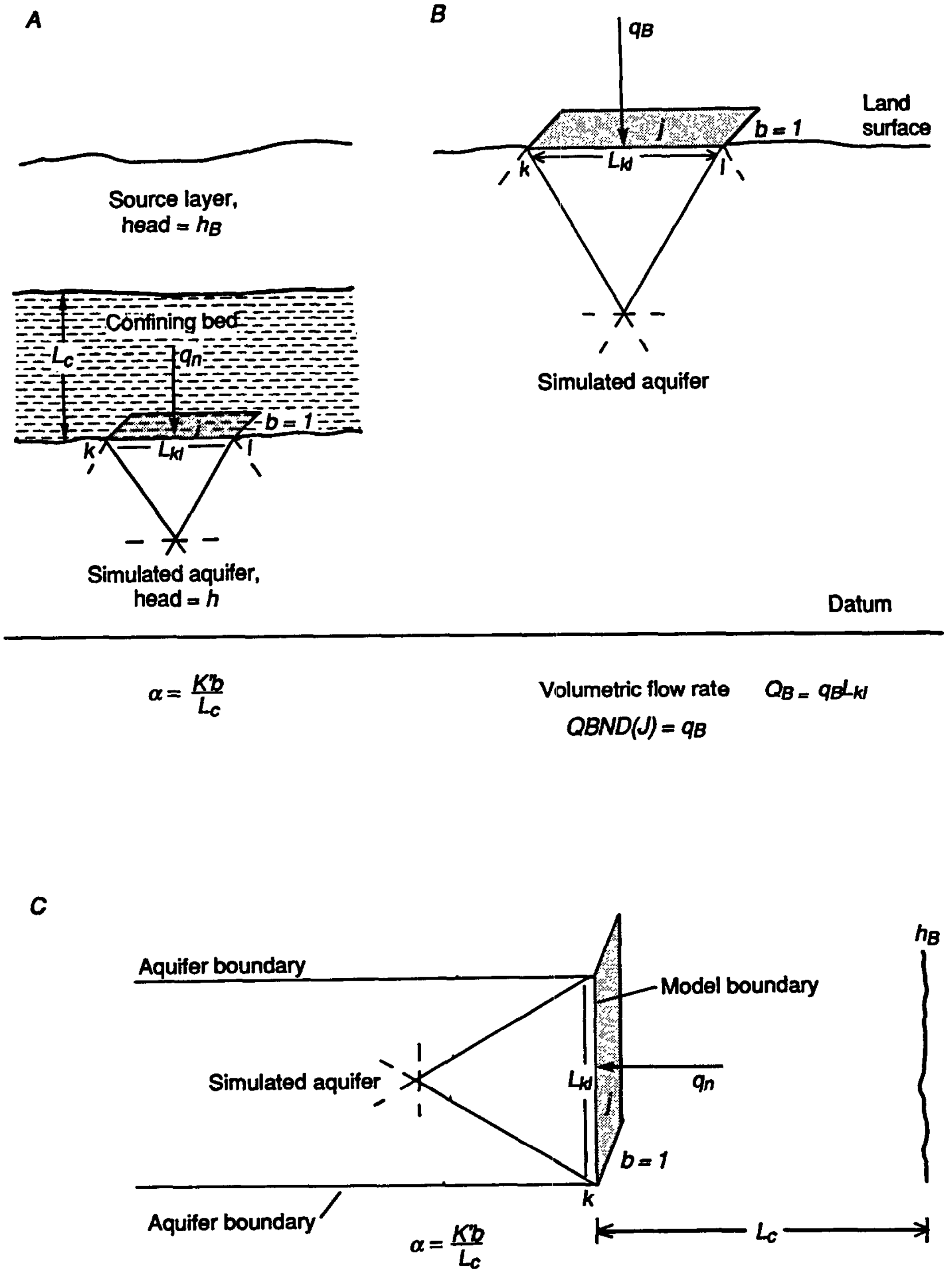


Figure 20.—Cauchy-type boundaries in aquifer cross sections for simulating (*A*) steady-vertical leakage; (*B*) areally distributed stresses; and (C) lateral flow across model boundaries.

Areally distributed stresses are represented in cross section as specified-flux boundaries along element sides (fig. 20*B*). The unit rate, W, in equation (1) is multiplied by the unit thickness of the cross section, b, to obtain the flow rate, q_B, per unit length across the element side. The volumetric flow rate, Q_B, is computed in MODFE by multiplying q_B by the length of the boundary side, L_{kl}.

As in the areal application of Cauchy-type boundaries, element sides that contain the same values of q_B

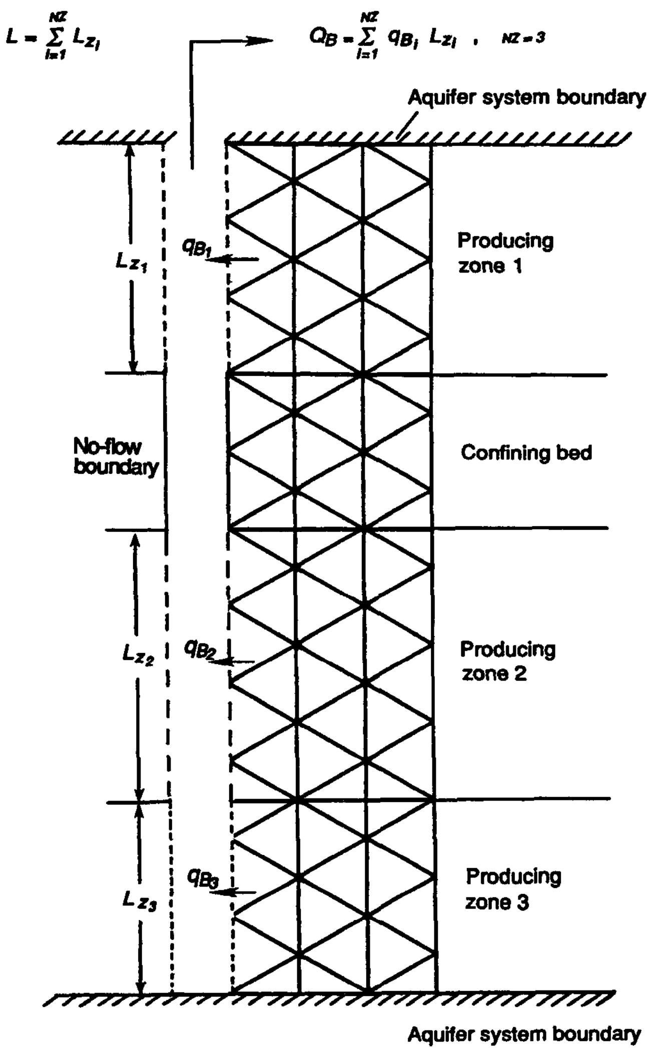


Figure 21.—Cross section of nonhomogeneous or multi-aquifer conditions showing flow to one well in the line of wells shown in figure 19*B* and application of specified-flux boundaries.

and α can be grouped together into one boundary-condition zone. Also, time variance of the boundary head H_B and of the unit flow rate q_B are permitted in cross-section simulations. Details of these features are given in the sections "Hydraulic-Property and Boundary-Condition Zones" and "Changing Stresses and Boundary Conditions With Time."

Axisymmetric Flow

An extension to cross-section simulations is the ability of MODFE to solve flow problems in axisymmetric-cylindrical (or radial) coordinates. A typical application is for simulating flow to a well, either in a single aquifer or in a layered system of aquifers and confining beds. As in cross-section simulations, transient-state, unconfined conditions involving a moving phreatic surface cannot be represented by axisymmetric flow with MODFE.

For axisymmetric-flow problems, the x axis is replaced by r, and y by z (fig. 22). The finite-element mesh is rotated about the z axis (r=0) so that each element represents a ring-like volume of material having a triangular cross section in the r-z plane (see figure 17 in Cooley, 1992). This rotation is not performed explicitly in MODFE; however, symmetry of the aquifer domain about the z axis is assumed. The concept of rotating the r-z plane about the z axis is necessary for identifying radial symmetry in field problems and for subsequent application of MODFE. The flow problem that is solved by MODFE is equivalent to a slice of aquifer material having a thickness of one radian, and is obtained by dividing the resulting equations by 2π (see following sections).

Axisymmetric flow implies that the aquifer material and boundary conditions are identical along any radius drawn from the z axis. Symmetry is assumed for hydraulic properties and boundary conditions about the line r=0, which is the z axis (fig. 22). For flow to a well, the line of symmetry is along the center of the well bore. Thus, element sides on the model boundary that is closest and parallel to the z axis, at $r=r_w$, trace the aquifer material in contact with the well bore. Similarly, zones for hydrologic properties and element sides representing boundary conditions, such as at $r=r_B$, are assumed to be rotated about the z axis. Because this rotation can produce many different shapes of hydrologic boundaries, care must be taken when designing the finite-element mesh for axisymmetric-flow as undesired boundary shapes can be formed.

Inputs for axisymmetric flow are analogous to those required for cross-sectional problems. The program variables XG and YG are used to represent radial (r) and vertical (z) node coordinates, respectively. The program variables XTR and YTR are used to input hydraulic conductivity in the radial and vertical directions, respectively, and specific storage is input as the program variable STR. The axisymmetric computations are invoked in MODFE by inputting a value of one (1) for the indicator variable IRAD.

Flow to a well and boundary conditions in axisymmetric flow can be represented in MODFE by using Cauchy-type boundary conditions. Applications of these boundary conditions to axisymmetric flow are given in the following sections. Details about these conditions are given in the sections "Specified Flux" and "Head-Dependent (Cauchy-Type) Flux."

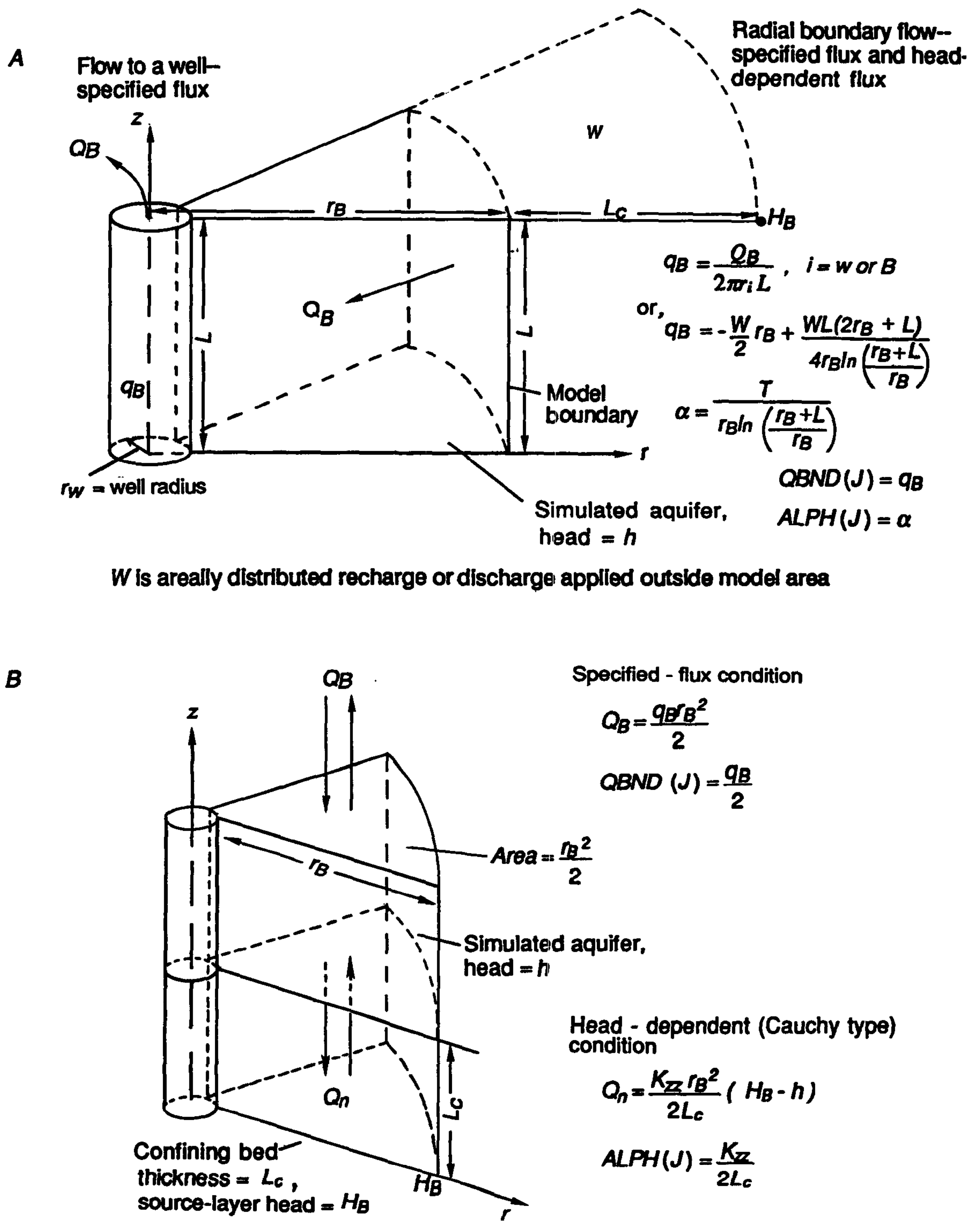


Figure 22.—Examples of Cauchy-type boundaries (specified flux and head-dependent flux) in axisymmetric flow for simulating boundary flow (*A*) in radial direction; and (*B*) in vertical direction.

Flow to a Well

Flow to a well in axisymmetric coordinates is represented in MODFE as a specified-flux boundary (fig. 22*A*). The specific discharge q_B [length/time] of the well is represented by the unit flow rate for the boundary condition, and is computed as

$$q_B = \frac{Q_B}{2\pi r_w L} \tag{4}$$

where Q_B is the volumetric flow rate [length^3/time], r_w is the well radius [length], and L is the length of screen or open hole to the aquifer. A nonzero well radius is required by MODFE; hence, the boundary length L cannot be located at the z axis. The denominator of equation (4) represents the cylindrical area of the boundary that results from rotation about the z axis. The 2π is factored out of Q_B because computations in MODFE represent a slice of the aquifer problem that is one radian thick.

As described previously for cross sections, the volumetric flow rate Q_B can be derived from one boundary zone of length L or from several boundary zones L_{zi} totalling L (fig. 21). In addition, each boundary zone can have a different unit flow rate q_{Bi}, corresponding to different producing zones in a nonhomogeneous aquifer or a multiaquifer system. These flow rates are computed for boundary zone i according to equation (4) by replacing q_B by q_{Bi}, L by L_{zi} and Q_B by Q_{Bi}, where Q_{Bi} is the known volumetric flow rate for the zone. Values of q_B or q_{Bi} are represented in MODFE as the program variable QBND(J) for each side j on the boundary.

Boundary Conditions Parallel to Z Axis

Boundary conditions that are parallel to and at a distance from the z axis in axisymmetric flow can be simulated by using Cauchy-type boundary conditions (fig. 22*A*). For a specified-flux boundary situated at a distance $r=r_B$ from the z axis, the unit flow rate q_B is computed in the same manner as for flow to a well by replacing r_w by r_B in equation (4). The term L in equation (4) is the length of the boundary across which the specified flux occurs, and Q_B is the volumetric flow rate. Care should be taken when applying this boundary condition as the specified flux is assumed to occur across the cylindrical area $2\pi r_B L$ that results from rotating r_B about the z axis.

A head-dependent (Cauchy-type) flux parallel to the z axis can be used to simulate flow across the outer boundary of the model area that results from stresses applied within the model area. This boundary condition usually supplies water to the model area in response to a pumped well located at $r=r_w$. Boundaries located at a distance r_B from the z axis are rotated in a manner similar to that of specified-flux boundaries and become boundaries having the cylindrical area $2\pi r_B L$, where L is the length of the boundary (fig. 22*A*). The unit flow rate normal to this cylindrical area is given by q_n, which is defined as in Cartesian coordinates by the product of the term α and the head difference $H_B - h$. The term α is computed as K_{rr}/L_c, where K_{rr} is the hydraulic conductivity of the material between the boundary and the external or boundary head, H_B, and L_c is the distance from the boundary to H_B.

Boundary Conditions Parallel to R Axis

Vertical flow across model boundaries parallel to the r axis in axisymmetric flow can be represented with Cauchy-type conditions. These boundary conditions represent areally distributed flow rates across the upper and lower (vertical) boundaries of the r-z plane because this plane is rotated about the z axis (fig. 22*B*). The specified-flux condition can be used to represent areally distributed stresses, such as applied recharge, constant rates of precipitation, or evapotranspiration. The head-dependent (Cauchy-type) condition can be used to represent steady vertical leakage or regional flow.

Because the axisymmetric-flow problem is represented in MODFE as a slice of aquifer material that is one radian thick, computations and data inputs for boundary conditions are affected by the factoring of 2π out of the model equations. For example, a vertical boundary of length r_B parallel to the r axis permits flow across the area of a circle of radius r_B, or πr_B^2. However, the area of one radian of arc (radius r_B) is $(\pi r_B^2)/2\pi$, or, $(r_B^2)/2$ (fig. 22*B*). Thus, the volumetric flow rate Q_B across a specified-flux boundary of length r_B is represented in MODFE as the flow across the area of one radian, or

$$Q_B = \frac{(q_B) r_B^2}{2} \tag{5}$$

where q_B is the unit recharge or discharge rate, which is identical to the W term of equation (1).

Values of $q_B/2$ are input to MODFE as the program variable QBND(J) for element side j along r_B. Most likely, more than one element side will be needed to represent r_B. For each side j on the boundary, Q_B is distributed proportionately according to the area that is created by rotating the side through one radian of arc.

For a head-dependent (Cauchy-type) boundary of length r_B, the volumetric flow rate across the area $r_B^2/2$ is given as

$$Q_n = \frac{(K_{zz}) r_B^2}{2L_c} (H_B - h) \qquad (6)$$

where K_{zz} is the vertical hydraulic conductivity of the material between the boundary r_B and the external head H_B located at a distance L_c from the boundary (fig. 22*B*). Values of $K_{zz}/2L_c$ are input to MODFE as ALPH(J) for boundary side j on r_B.

Although values for ALPH(J) and QBND(J) can vary for element sides on a Cauchy-type boundary, symmetry of the axisymmetric-flow problem may prevent different values for these boundary terms from being used. Boundary-condition zones represent concentric-circular areas about the z axis, and each zone can be assigned distinct values for ALPH(J) or QBND(J). However, the geometric configuration of concentric rings of aquifer material, each containing different values for Cauchy-type boundaries, may not represent the true distribution of boundary conditions for the aquifer problem. Therefore, boundary-condition zones should be selected carefully for axisymmetric-flow problems.

Water-table (Unconfined) Conditions

Two-dimensional ground-water flow in a water-table (unconfined) aquifer that is assumed to be governed by the nonlinear form of equation (1) can be simulated by MODFE. The flow is nonlinear because the effective aquifer transmissivity is a function of the saturated aquifer thickness, which changes as the hydraulic head changes during the simulation. The aquifer-storage characteristics also may be nonlinear if, during the simulation, the aquifer converts from confined to unconfined conditions or from unconfined to confined conditions. However, for water-table conditions without conversion, the aquifer-storage properties are assumed to be constant in time and are defined by the specific yield. Changes in aquifer-storage properties are discussed in the section "Conversion Between Confined and Unconfined Aquifer Conditions."

The variation in transmissivity with time is represented in MODFE by a predictor-corrector technique that approximates hydraulic head at the advanced time level. Details of this technique are given in the section "Unconfined Flow," in Cooley (1992). In general, head changes that are computed during the predictor step are used to obtain estimates of aquifer thickness and transmissivity for the corrector step. The corrector step solves the finite-element equations for head changes over the same time level as the predictor step. Head changes during the corrector step are caused by using different transmissivity values from those used during the predictor step. Updates to aquifer thickness and transmissivity for the advanced time level are based on head changes from both steps.

The ability of the predictor-corrector technique to approximate the time variance in aquifer thickness and transmissivity is related to the size of the time-steps used to subdivide the simulation period. Inappropriately large time steps usually increase the errors associated with approximating thickness and transmissivity during the simulation. Approximation errors are manifested in model results as large flow imbalances in the water-balance summary and as incorrect values of computed water levels. However, using time steps that are too large for the nonlinearity imposed on the aquifer problem by water-table conditions may not be the only cause of large flow imbalances and an incorrect solution. Errors associated with improper use of boundary conditions or inaccurate specification of hydraulic properties also contribute to inaccuracies in the model results, and determining the cause of errors in model results may be a difficult task. The effects of the time-step size on the approximation of aquifer thickness and transmissivity and on the flow imbalance are discussed in the sections "Water-table (Unconfined) Conditions" and "Water-Balance Summary and Flow Imbalance" in Torak (1993).

To solve water-table problems by using MODFE, the user must structure the main program to contain subroutines that perform the water-table computations and the predictor-corrector technique. Details on structuring MODFE and diagrams showing program structures for steady-state and nonsteady-state water-table versions are given in the section "Program Structures and Lists of Main Programs" in Torak (1993). Programming details of the water-table computations are given in the section "Water-table (Unconfined) Conditions" in Torak (1993).

Inputs to MODFE for water-table simulations consist of values for hydraulic conductivity, altitude of the top of the aquifer, aquifer thickness, and specific yield (fig. 23). Hydraulic conductivity is represented with program variables XTR and YTR for the x and y directions, respectively, and is input by hydraulic-property zone. Aquifer thickness and the altitude of the aquifer top are input by node and are represented, respectively, by program variables THK and TOP. Nodal values for TOP are selected as either the altitude of land surface or the altitude of the base of an overlying confining bed. Specific yield is represented by program variable SY and is input by aquifer-property zone. Aquifer storage coefficient also is required as input for simulations involving conversion between confined and unconfined conditions. The storage coefficient is represented as program variable

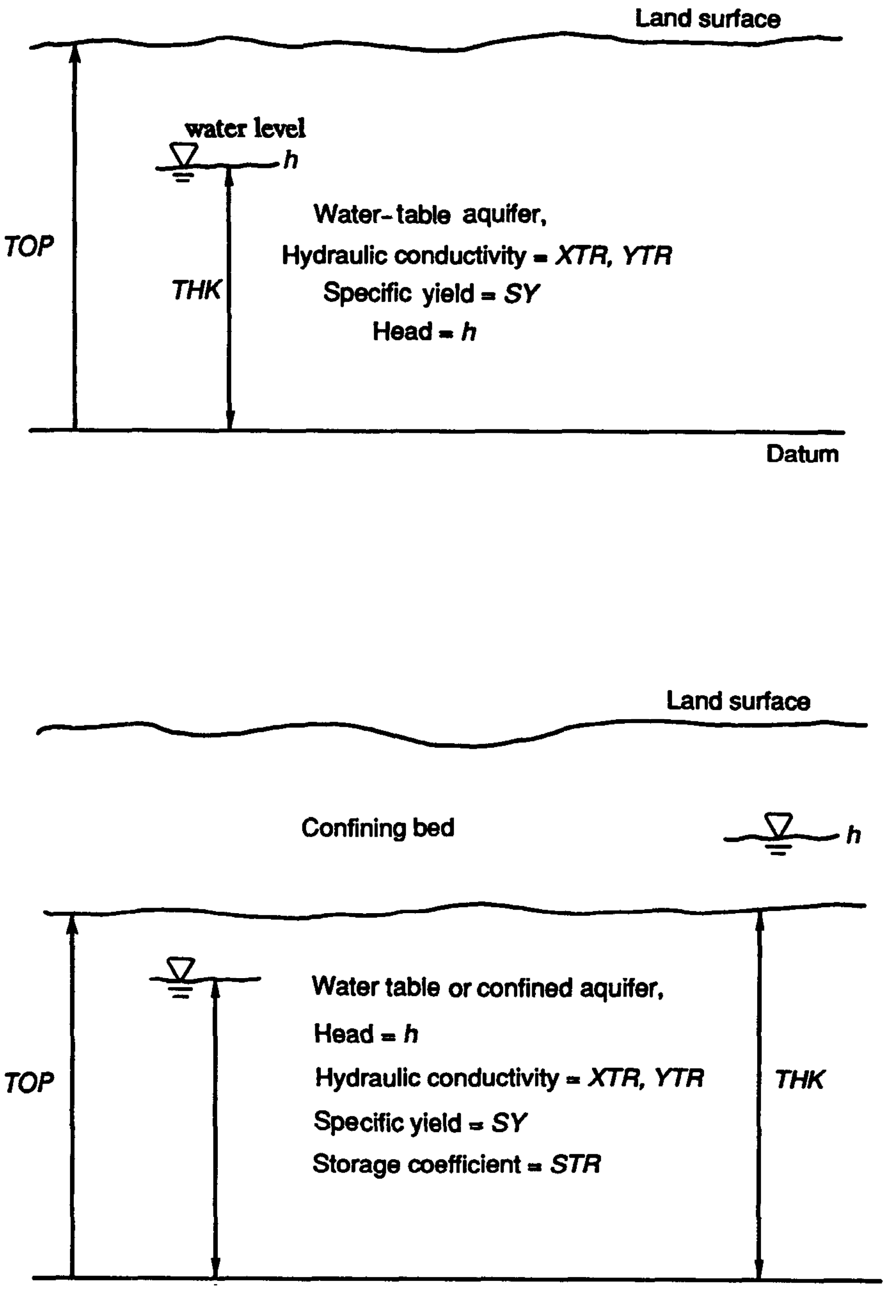


Figure 23.—Water-table aquifer conditions and nomenclature used in MODular Finite-Element model (MODFE).

STR. Details about data inputs are contained in the section "Input Instructions."

Simulations that cause inundation of land surface by rising ground-water levels from a surficial aquifer also will cause conversion from unconfined to confined conditions. This is because the nonsteady-state water-table versions of MODFE formulate aquifer conversions automatically regardless of whether or not an overlying confining bed is present. Conversion (and inundation) occurs for a surficial aquifer when the aquifer head exceeds the value of TOP at a node. For this case, the value of TOP represents land surface altitude, which is compared with aquifer head, H, to update thickness and change aquifer-storage terms at each node. Although inundation may not be the desired simulation result, conversion of storage terms can be avoided when inundation occurs by setting values of aquifer storage coefficient, program variable STR, equal to the specific yield, SY, on input, for water-table simulations. If inundation of land surface

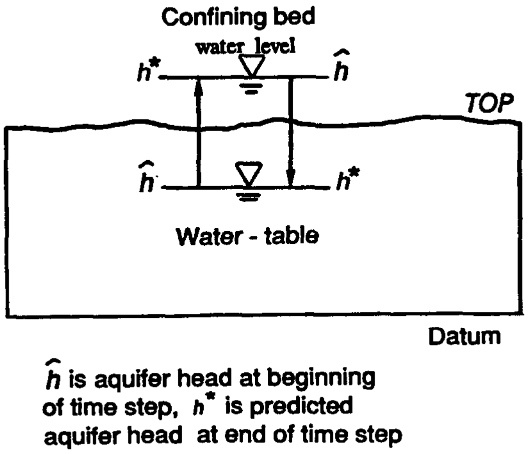


Figure 24.—Configuration of aquifer head and altitude of base of overlying confining bed (*TOP*) for conversion between confined and unconfined conditions.

is the intended result, then the value input for STR would be somewhat larger than the value of specific yield. However, use of MODFE for inundation-type problems should proceed with care because the storage-conversion formulation in MODFE was not designed for this application, and overland flow is not simulated for the inundation condition.

Conversion Between Confined and Unconfined Aquifer Conditions

For certain ground-water-flow problems, the aquifer head may be above the altitude of the base of an overlying confining bed (confined conditions) at one instant in time, only to drop below the base of the overlying confining bed at another instant in time (unconfined conditions). Conversely, the aquifer head may be below the altitude of the base of an overlying confining bed at one time, only to increase above the base of the overlying confining layer at later time (fig. 24). These configurations of aquifer head and altitude of the base of an overlying confining bed describe the conversion of an aquifer between confined and unconfined conditions. Conversion causes changes in the manner in which water is released or accumulated by aquifer storage as the confined storage coefficient is smaller than the specific yield of a water-table aquifer by at least two or three orders of magnitude. Computations are performed in MODFE to account for the effects on computed hydraulic head of changing aquifer storage properties during conversion.

Computations that allow aquifer conversion between confined and unconfined conditions are performed automatically in the nonsteady-state water-table versions of MODFE. Details of structuring the main program for water-table simulations are given in the section "Program Structures and Lists of Main Programs" in Torak (1993). The nonsteady-state water-table versions of MODFE use the predictor-corrector technique to approximate aquifer thickness and transmissivity during the simulation. Checks are made on the hydraulic head at each node at the beginning of a time step and at the end of the predictor step to determine whether aquifer conversion had taken place (fig. 24). Aquifer conversion occurs when the head at a node rises above or drops below the altitude of the base of an overlying confining bed during a time step (represented as TOP in fig. 24). Details of the computations of aquifer thickness and storage at nodes that experience aquifer conversion are given in the section "Conversion Between Confined- and Unconfined-Aquifer Conditions" in Torak (1993).

The inputs required to simulate conversion between confined and unconfined aquifer conditions are the same as those described for water-table simulations (see previous section and fig. 23.). Values for the confined storage coefficient and the specific yield are input for aquifer-conversion problems. The storage coefficient is represented in MODFE as the program variable STR, and the specific yield is represented as the program variable SY. The altitude of the base of the overlying confining bed is input as the variable TOP. Details of inputs for water-table simulations and for aquifer conversions are given in the section "Input Instructions."

Drying and Resaturation of Aquifer Material

A water-table aquifer may respond to stresses and boundary conditions by drying (desaturating) along its external boundaries, such as a surficial aquifer of valley-fill deposits in contact with bedrock-valley walls (fig. 25), or by localized drying within the aquifer region, such as in the vicinity of a pumped well. Conversely, stresses and boundary conditions may be such that dry aquifer material may become saturated, or resaturated, after a period of desaturation (dryness). Conditions of drying and resaturating parts of a water-table aquifer are simulated automatically in the water-table versions MODFE. The drying condition is represented in MODFE as a zero or negative value of aquifer thickness (program variable THK) at a node.

Negative values of aquifer thickness enable the water-table to pull away from the dry node and the element to become partially dewatered (fig. 26). Because the head at the dry node is allowed to drop below the base of the aquifer, hydraulic gradients within the partially dry element and within neighbor-

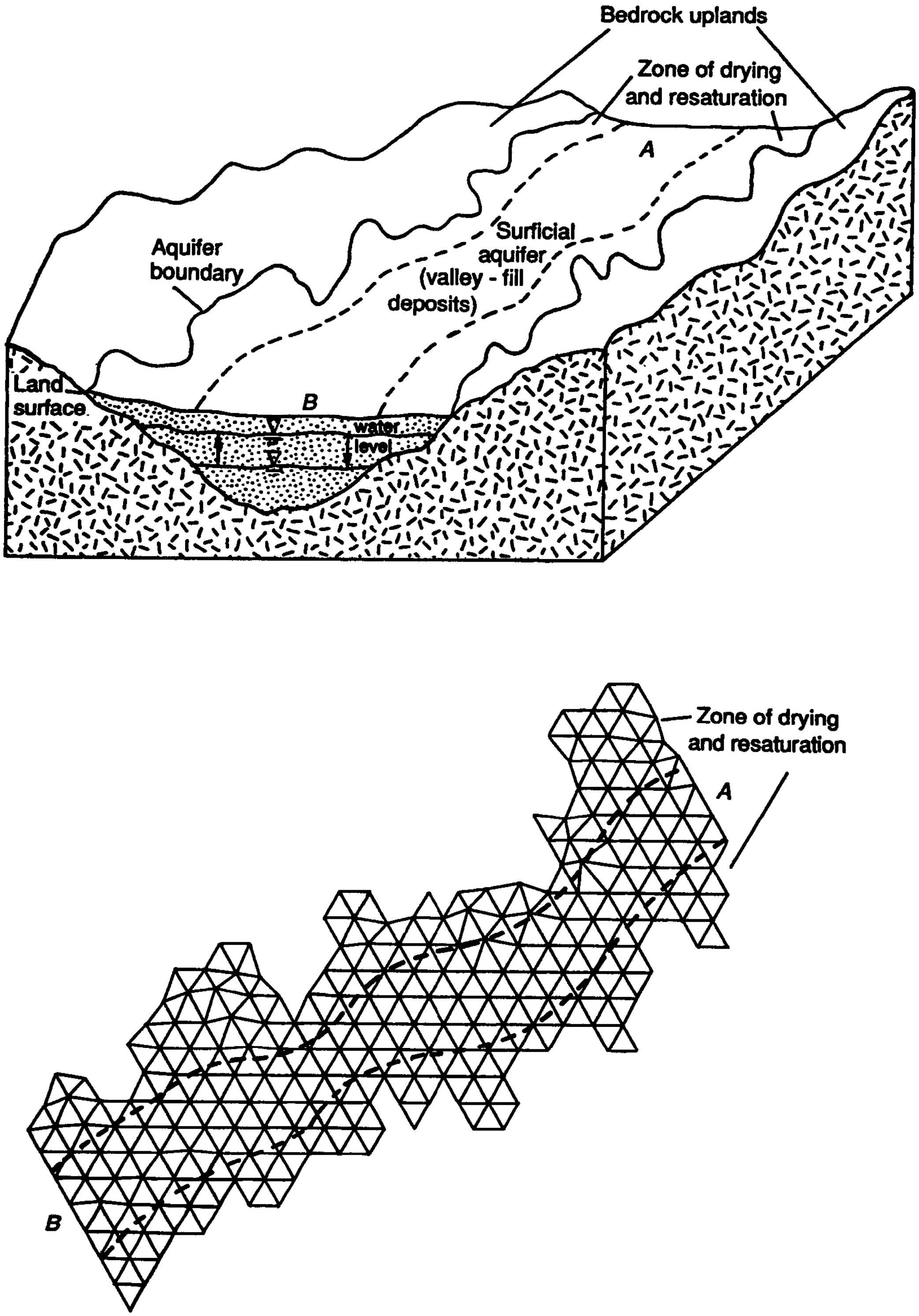
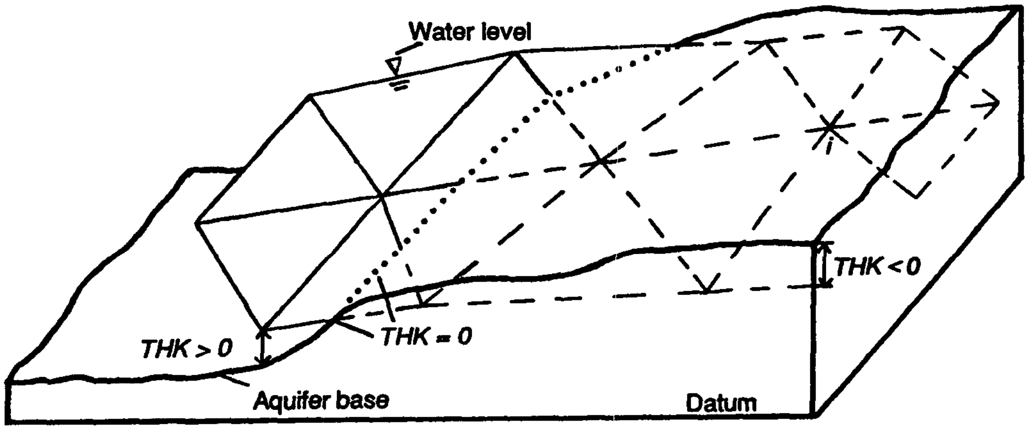


Figure 25.—(*A*) Block diagram of surficial aquifer (valley-fill deposits) bounded by bedrock uplands; and (*B*) finite-element mesh used to simulate drying and resturation of aquifer material.



Aquifer thickness represented by *THK*
***THK* ≤ *0* indicates dewatering.**
Dashed line indicates dry or partially dry element side.
Node *i* in center of patch of dry elements

Figure 26.—Potentiometric surface of water-table aquifer, subdivided by finite-elements, showing drying conditions.

ing elements can remain nearly horizontal during the drying process. This configuration of aquifer head may represent a more realistic hydrologic condition than if head at the dry node were fixed at the base of the aquifer during drying. Negative thickness values at dry nodes are not used in computations; however, they are used to determine the amount of head increase that is needed to resaturate the aquifer at the dry node.

A dry node continues to be part of the flow system, and head changes continue to be computed there, as long as the node is linked to nondry nodes or as stresses at the dry node indicate recharge conditions. Resaturation occurs when boundary conditions, lateral flow, or stresses allow water levels to increase to the point where head changes at the dry node cause a positive value of aquifer thickness to be computed.

Head changes are not computed at dry nodes that are completely surrounded by other dry nodes, thus creating a patch of dry elements (fig. 26). For this condition, resaturation can occur only if a node that is linked to the center of a patch of dry elements becomes resaturated. Thus, the dry node in the center of the patch becomes linked to nondry nodes in the model area and can resaturate. Details of the equation development for dry nodes are given in the section "Drying and Resaturation of Nodes" in Cooley (1992). Programming details are given in the section "Aquifer Drying and Resaturation" in Torak (1993).

Drying and resaturation are nonlinear processes that require the predictor-corrector technique to update aquifer thickness during a time step. To assist the user in keeping track of dry nodes during simulation, the following message is printed out from the corrector step:

```
NODE ___ PREDICTED TO BE DRY
PREDICTED AQUIFER THICKNESS AT NODE =___
NET FLOW AT NODE =___
```

where the appropriate values for the node number, aquifer thickness, and sum of known flows at the dry node are printed in the blank spaces. If the net flow at a dry node is negative, indicating discharge, then, obviously, ground water cannot be extracted from the aquifer at that rate. In an attempt to simulate a more realistic aquifer problem by keeping the node from going dry, the discharge rate is decreased by half of its current value and a message is printed out stating that this has occurred. The decreased discharge rate is used at the dry node for the corrector step and for subsequent time steps or iteration levels, even if the node remains saturated. If the node is predicted to go dry on the time step or iteration level following a decrease in discharge, then the discharge rate is decreased again by half of its current value. The decrease in discharge rate by half is completely arbitrary. The printed message alerts the user of the dry node so that this condition can be evaluated after the simulation. The user can consult the programming details in the section "Aquifer Drying and Resaturation" in Torak (1993) to modify the program as needed to provide other consequences of drying at a node containing a net discharge rate, such as decreasing the discharge rate by an amount other than one half, not decreasing the discharge rate, or stopping MODFE.

Nonlinear Head-Dependent Flux

Boundary conditions containing head-dependent (Cauchy-type) fluxes and steady vertical leakage usually are linear; that is, the volumetric flow rate is proportional to a head difference, and the mathematical expression defining the boundary condition is fixed for all values of aquifer head (see sections "Head-Dependent (Cauchy-Type) Flux" and "Steady Vertical Leakage"). However, for some aquifer problems, the flow rate from these conditions can be limited to a maximum or minimum value depending on the position of the aquifer head relative to a controlling head or altitude. These limitations require that the mathematical expression for the boundary condition change depending on evaluation of the aquifer head with the controlling head or altitude. Because the form of the mathematical expression defining the boundary condition can change as the aquifer head changes, the boundary condition and the functions used to describe them are nonlinear. Some examples of nonlinear head-dependent fluxes are: (1) flow across a riverbed when the water-table drops below the altitude of the bottom of the riverbed sediments, (2) flow to or from an overlying fault or fracture zone or an overlying source layer (steady vertical leakage) when the aquifer converts between confined and unconfined conditions, (3) spring discharge or irrigation drainage, and (4) evapotranspiration.

The following sections describe the application of nonlinear head-dependent functions for simulating nonlinear boundary conditions such as those listed above. The mathematical representation of nonlinear boundary conditions in MODFE permits many more applications than those just given. Consequently, the nonlinear head-dependent functions are categorized as Cauchy type, point sinks, and steady vertical leakage instead of as rivers, springs, and evapotranspiration, respectively.

Simulation of nonlinear head-dependent flux requires use of the nonlinear versions of MODFE, which contain either the predictor-corrector technique for nonsteady-state conditions or an iterative method for steady-state conditions. The computations for nonlinear head-dependent (Cauchy-type) functions and nonlinear point sinks are contained in a set of subroutines that begin with the letters GN. These subroutines and their call statements are added to the program structure by the user if these simulation capabilities are needed. The computations for nonlinear steady vertical leakage are contained in a similar set of subroutines beginning with the letters VN. Instructions for incorporating nonlinear head-dependent functions into MODFE are given in the section "Program Structures and Lists of Main Programs" in Torak (1993).

Cauchy Type

The nonlinear form of the head-dependent Cauchy-type boundary can be used to compute flow rates across line-oriented boundaries that are limited to a maximum or minimum value by a controlling head or altitude. Examples of hydrologic features that can be simulated by using this boundary condition are similar to those given for the linear case, and include flow across a riverbed, fault or fracture zone, or a model boundary (see figs. 16–18, and 20). For simulating flow across a riverbed, the flux is limited to a maximum inflow rate to the aquifer when the aquifer head h drops below the altitude of the bottom of the riverbed sediments z_r (fig. 27*A*). The flux across a fault or fracture zone that is situated in a confining bed overlying an aquifer is limited to a maximum inflow rate when the aquifer undergoes conversion from confined to unconfined conditions (fig. 27*B*). Flow to an irrigation drain or slough can be limited so that only discharge from the aquifer occurs when the aquifer head rises above the altitude of the feature (fig. 27*C*). Other applications in areal or cross-sectional dimensions may limit the flux to a maximum rate depending on aquifer geometry or the flow problem to be solved.

The expression for the flux across a nonlinear head-dependent (Cauchy-type) boundary is given by equation (152) in Cooley (1992). The head or altitude that limits the flow rate is represented by the term z_r. The boundary or external head is given by H_r and is analogous to H_B in equation (6) for a (linear) head-dependent (Cauchy-type) boundary. The term α_r is analogous to the α term in equation (6) (see the discussions of α and H_B in the section "Head-Dependent (Cauchy-Type) Flux" for descriptions of these terms).

Definitions of H_r and z_r vary depending on the application of the nonlinear boundary condition. For simulating flow across a riverbed, H_r is the altitude of the river stage and z_r is the altitude of the bottom of the riverbed sediments (fig. 27*A*). To simulate flow through a fault or fracture zone, z_r is the altitude of the base of the zone in the overlying confining bed, and H_r is the source-layer head or other head that governs the flow rate through the zone (fig. 27*B*). To simulate a discharge-only boundary, such as a drain, z_r is the altitude of the drain and H_r is set equal to z_r (fig. 27*C*).

Like H_r and z_r, the term α_r is defined according to the particular application of the nonlinear boundary

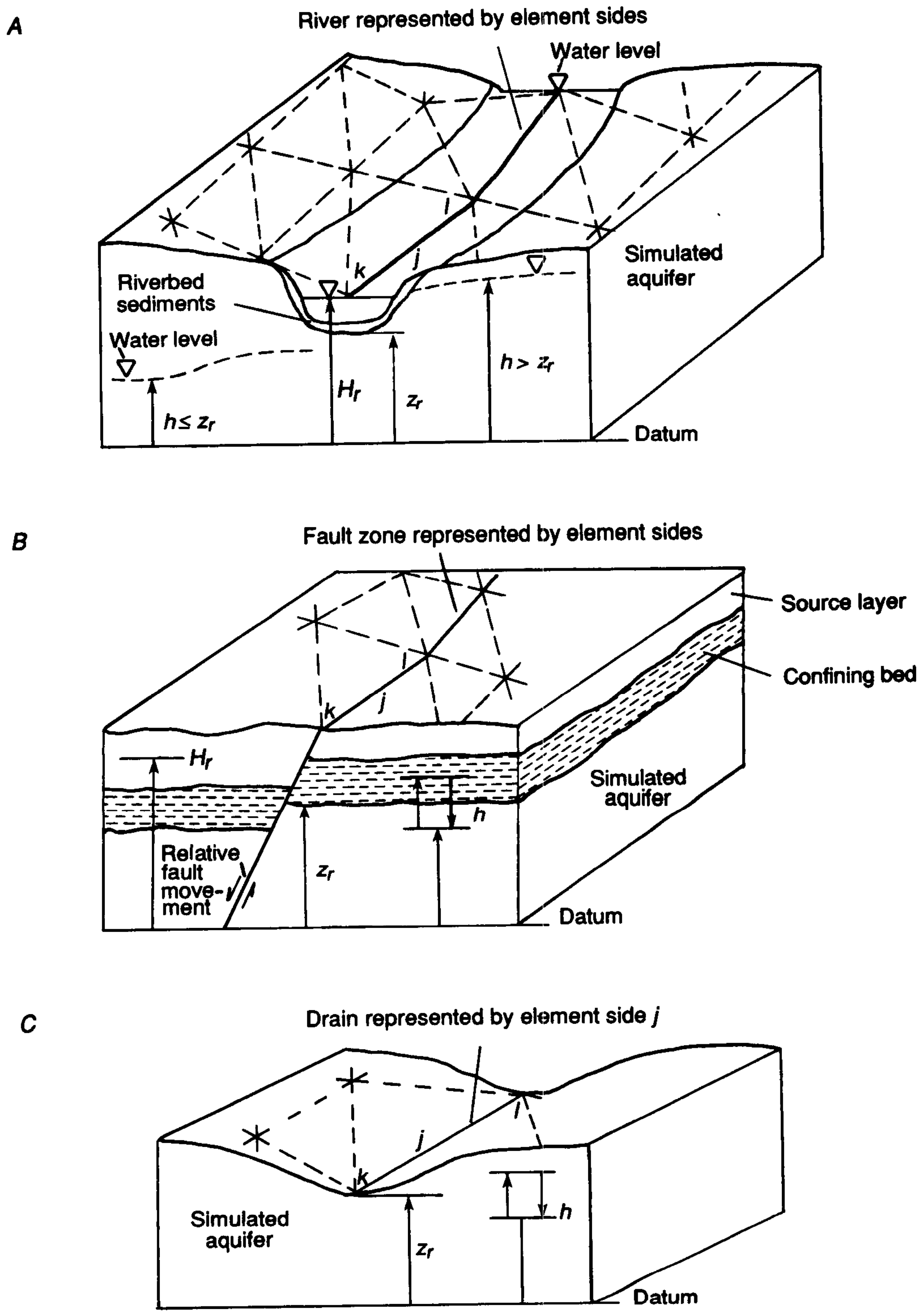


Figure 27.—Nonlinear head-dependent (Cauchy-type) boundaries simulating (*A*) flow across a river bed; (*B*) flow along a fault zone; and (C) flow to an irrigation drain.

condition. For simulating a river, fault or fracture zone, or boundary flow, α_r is identical to the α term defined previously for simulating these features by the linear boundary condition (see section "Head-dependent (Cauchy-type) Flux"). For simulating a drain, α_r is assigned values that relate the hydraulic characteristics of the drain (geometry, aperture or diameter of the opening (if applicable), material type, etc.) to the flow rate. Usually, values for α_r are adjusted during calibration until the computed flow rate matches the observed drain discharge.

Inputs for nonlinear head-dependent (Cauchy-type) boundaries consist of nodal values of H_r and z_r, node numbers defining the boundary, and values of α_r for each element side on the boundary. Before inputting these values, the number of boundary sides and zones are input, respectively, as the program variables NBNC and NLCZ. These values are used to allocate computer storage for program variables associated with this boundary condition. The following variables are used to input terms for the nonlinear head-dependent (Cauchy-type) boundaries at nodes k and l, respectively, on boundary side J (fig. 27): node numbers are input as KR(J) and LR(J); boundary or external head H_r is input as HRK(J) and HRL(J); and the controlling head or altitude is input as ZRK(J) and ZRL(J). Additional descriptions of these data inputs are given in the section "Input Instructions."

The α_r term is input by boundary side as the program variable GC(J). Boundary sides that have the same value of α_r can be grouped into one boundary-condition zone for input. Details of establishing boundary-condition zones are given in the section "Hydraulic Property and Boundary-Condition Zones." A time-varying boundary condition can be represented in MODFE by changing values for H_r during the simulation. Typical applications are for changing river stages and source-layer heads with time. Details about changing H_r with time are given in the section "Changing Stresses and Boundary Conditions with Time."

Point Sinks

Hydrologic features that create nonlinear head-dependent discharge at point locations in an aquifer can be represented with the nonlinear head-dependent flux called point sinks. These boundary conditions are represented by nodes in the finite-element mesh. Typical applications of nonlinear point sinks are for representing springs and irrigation drains (fig. 28), where the hydrologic conditions permit only discharge from the aquifer. The flux out of the aquifer is zero if the aquifer head, h, is below the reference altitude z_p; thus, discharge occurs only for cases where h is greater than z_p. For springs, z_p is the altitude of the discharge point in the aquifer (fig. 28*A*). For irrigation drains, z_p is the altitude of the drain opening (fig. 28*B*).

The volumetric flow rate from nonlinear point sinks is expressed in equation (106) in Cooley (1992) as the product of a discharge coefficient, C_{pi}, and the head or altitude difference $(z_{pi} - h_i)$, for node i. The term C_{pi} is analogous to α_r, described in the previous section, for the case where the nonlinear head-dependent (Cauchy-type) boundary represents a discharge-only function. Values for C_{pi} relate the head difference to the volumetric discharge rate and represent the hydraulic characteristics of the spring or drain opening. Usually, the values of C_{pi} are adjusted during calibration until the computed discharge rates match the observed values.

Inputs for nonlinear point sinks consist of the node number where the boundary is located, the reference elevation, z_p, and the value of the discharge coefficient. The number of each boundary node, i, is represented by program variable KP(I), and the reference altitude, z_{pi}, is given by HZP(I). The discharge coefficient, C_{pi}, is represented by program variable GCP. In addition to these inputs, the number of point sinks is input as program variable NPNB and is used to allocate storage for terms associated with this boundary condition. Details about these data inputs are given in the section "Input Instructions."

Steady Vertical Leakage and Evapotranspiration

A nonlinear form of the steady vertical leakage term $R(H - h)$ in equation (1) can be used to limit the head-dependent flux to a maximum recharge or discharge rate over an area or subarea of the aquifer. Some examples of nonlinear steady vertical leakage are: (1) leakage across a confining bed overlying an aquifer that converts between confined and unconfined conditions, (2) leakage through surface-water sediments, such as through a riverbed, when the feature is represented by elements instead of by element sides, and (3) evapotranspiration (fig. 29). For leakage across a confining bed, the head-dependent flux is limited to a maximum inflow (recharge) rate when the aquifer head h is below the altitude of the bottom of the overlying confining bed, z_t (fig. 29*A*). The head-dependent flux across sediments beneath a wide river or lake is limited to a maximum inflow rate when the aquifer head is below the altitude of the bottom of the sediments (fig. 29*B*).

The nonlinear head-dependent flux representing evapotranspiration is a discharge-only type, and is analogous to point sinks or drains, discussed in the previous sections. The evapotranspiration rate, S_e, is

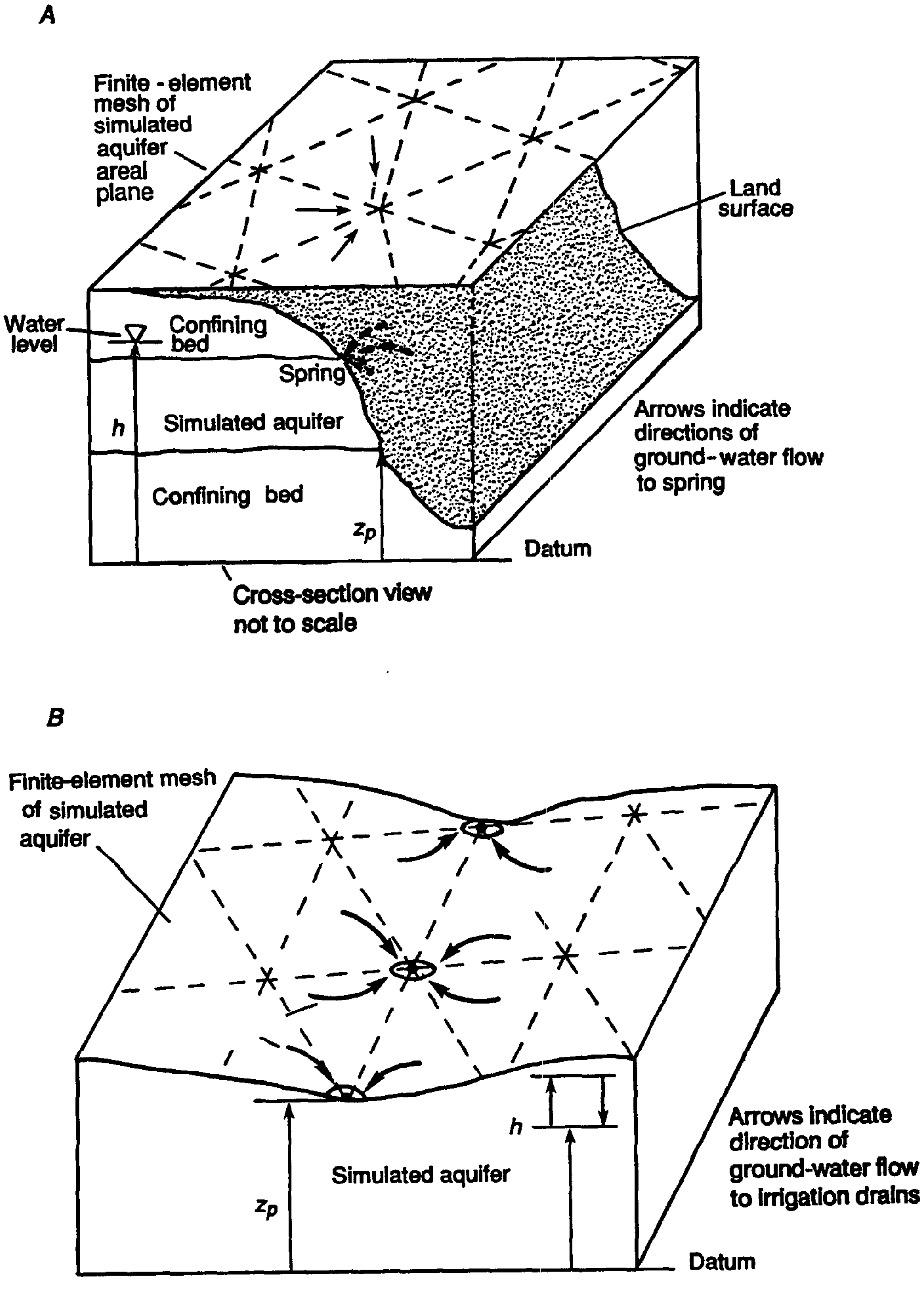


Figure 28.—Nonlinear head-dependent point sinks simulating (*A*) spring at node *i* and (*B*) irrigation drains.

assumed to vary linearly when the aquifer head, h, is situated between land surface and the altitude, z_e, below which the rate is zero. The depth below land surface where S_e is zero is called the extinction depth, d_e. These terms are depicted in figure 29*C*. Evapotranspiration (discharge) occurs at a maximum rate, S_e(max), when the aquifer head equals or exceeds land surface, and is zero when the aquifer head is below z_e,

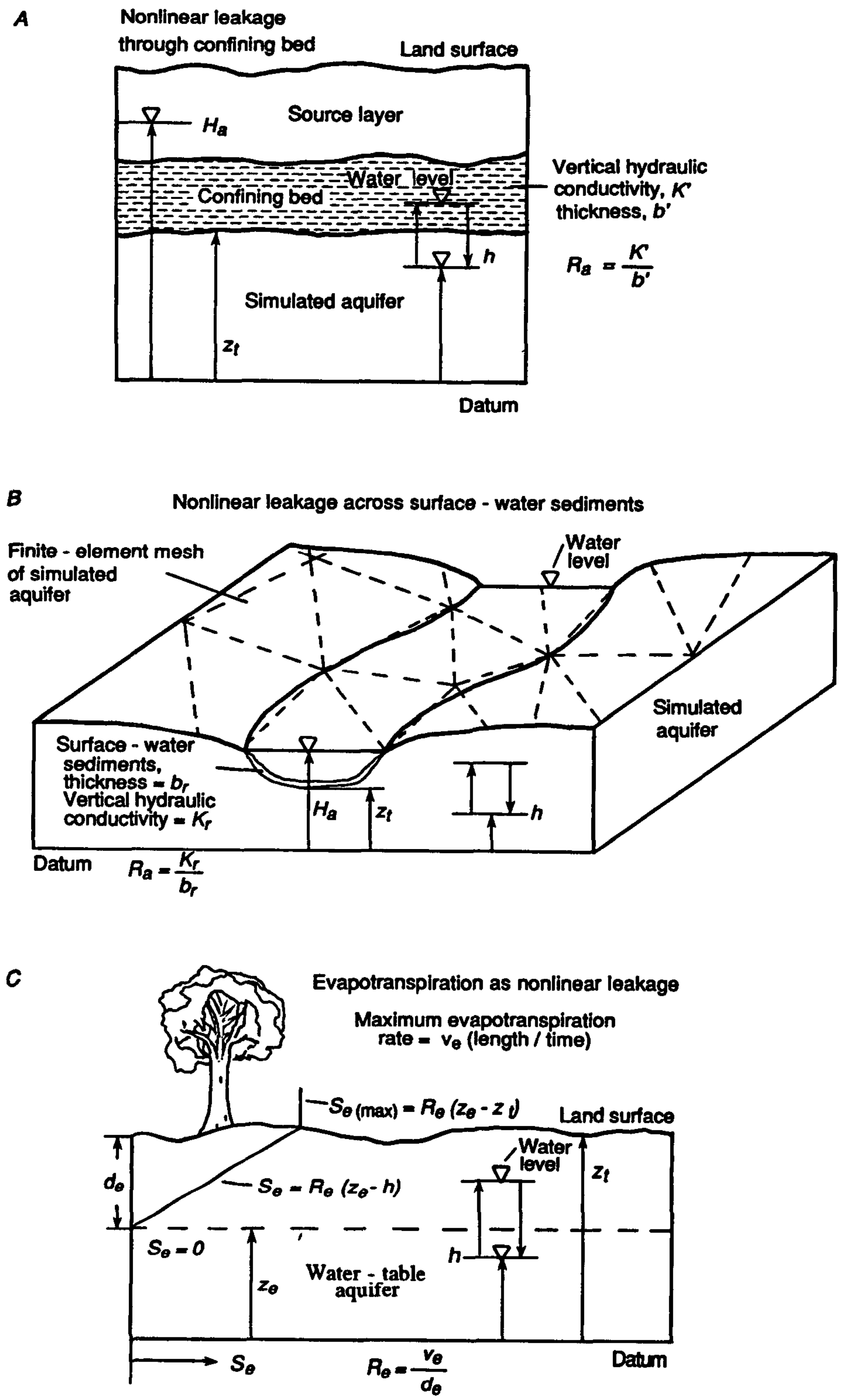


Figure 29.—Nonlinear steady vertical leakage simulating (*A*) flow through confining bed; (*B*) flow across riverbed sediments; and (*C*) evapotranspiration.

which may be the bottom of the root zone. The user may modify the equation-forming subroutine for nonlinear steady vertical leakage if other than linear variation of the evapotranspiration rate with depth below land surface is to be represented. Programming details of the nonlinear head-dependent fluxes are described in Torak (1993).

The expressions for nonlinear steady vertical leakage are given by equation (117) in Cooley (1992), for cases where the maximum inflow rate is limited (examples 1 and 2, above), and by equation (128) in Cooley (1992), for cases where the flux is a discharge-only type (example 3). The terms R_a and R_e, which relate the head differences to the flow rates in these equations, are analogous to the hydraulic conductance R in equation (1) for steady vertical leakage. R_a is computed as the vertical hydraulic conductance of the confining bed or the surface-water sediments; that is, vertical hydraulic conductivity divided by thickness (fig. 29*A*,*B*). R_e is computed as the maximum unit discharge rate, v_e, such as -30 inches/year, divided by the depth interval, d_e (fig. 29*C*). The negative sign is used in the computation of R_e and in the value that is input to MODFE in order to distinguish between the two types of nonlinear steady vertical leakage in the program.

The definition of heads or altitudes that control the nonlinear steady vertical leakage varies depending on the application of the boundary condition. The source-layer head or surface-water level is represented as H_a (fig. 29*A*,*B*). The altitude of the base of the operating zone for the discharge-only function is given as z_e (fig. 29*C*). The altitude of the base of the overlying confining layer or of the surface-water sediments and land surface is defined as z_t.

To simulate nonlinear steady vertical leakage, the area containing the flux is discretized by elements and identified by a unique boundary-condition zone. Details about creating boundary-condition zones are given in the section "Hydraulic Property and Boundary Condition Zones." Elements within a zone can simulate either the condition in which the flux is limited to a maximum rate (examples 1 and 2) or the discharge-only condition (example 3).

Inputs for nonlinear steady vertical leakage consist of the conductance terms R_a or R_e and the controlling heads or altitudes H_a, z_e, and z_t. The conductance terms are represented in MODFE as the program variable VNCF (with negative values for R_e) and are input by boundary-condition zone. The source-layer head or surface-water level H_a and the altitude of the extinction depth z_e is represented by program variable HS, and is input by node. Because nonlinear steady vertical leakage is formulated by using the water-table versions of MODFE, the input of program variable TOP for water-table simulations is used for the altitude of land surface or base of the overlying confining bed, z_e. Thus, nodal values for z_e are not input specifically for this boundary condition. A description of the inputs for nonlinear steady vertical leakage is given in the section "Input Instructions."

Values of the controlling head HS are permitted to change during the simulation to represent a time-varying boundary condition. This feature is useful for varying, for example, surface-water levels or the extinction depth of evapotranspiration to account for seasonal fluctuations in water levels or changes in the ground-water demand by vegetation, respectively. Details of changing HS with time are given in the section "Changing Stresses and Boundary Conditions with Time."

Steady-State Flow

MODFE can be used to solve the two-dimensional ground-water-flow equation (1) for hydraulic heads under steady-state conditions. As discussed in Cooley (1992), steady-state conditions exist, theoretically, when the time derivative of hydraulic head in equation (1) is zero. This causes the storage term $S\partial h/\partial t$ to drop out of the equation and ground-water flow to be independent of aquifer storage and time. The steady-state solution also is independent of the initial conditions of hydraulic head, but requires at least one specified-head boundary (node) or a head-dependent (Cauchy-type) boundary with the nonzero α coefficient to obtain a unique solution.

Because initial estimates of hydraulic head may differ greatly from the actual solution, nonlinear-flow conditions can be simulated prior to achieving a steady-state solution. Examples of nonlinear steady-state-flow problems are water-table (unconfined) conditions, drying or resaturation of parts of the aquifer region, and nonlinear head-dependent flux. These types of aquifer problems are solved by using nonlinear steady-state versions of MODFE, which differ in program structure from the nonlinear, nonsteady-state versions. Linear-flow problems, such as confined conditions with linear boundary conditions are solved by using the linear versions of MODFE, which can solve steady- and nonsteady-state problems. Linear and nonlinear versions of MODFE are listed in Tables 4–6 in the section "Input Instructions" according to their simulation capabilities. Program structures for linear and nonlinear steady-state versions of MODFE are given in the section "Program Structures and Lists of Main Programs" in Torak (1993). Inputs and other information about linear and nonlinear steady-state conditions are discussed in the following sections.

Linear Conditions

Inputs to the linear versions of MODFE determine whether steady- or nonsteady-state conditions are formulated within the program. Steady-state computations are initiated by entering a value of one (1) for the indicator variable ISTD. All values for storage coefficient or specific yield (program variables STR and SY, respectively) are input as zero or left blank. A single time step having a value of one (1.) is required for steady-state simulations. Although steady-state flow is independent of time, a time-step size of one ensures that division by zero will not take place in the equation-forming subroutines, and that values computed for the water-balance summary represent volumes for a unit-time interval. Details of these and other data inputs are given in the section "Input Instructions."

Nonlinear Conditions

Nonlinear conditions of steady-state ground-water flow are represented in MODFE by an iterative-solution method that contains data inputs and equation formulations that differ from the nonlinear, nonsteady-state versions. The iterative method contains water-table iterations during which aquifer thickness and terms associated with nonlinear boundary conditions are updated by using head changes from the previous (or initial) iteration level. Details of the iterative scheme and of these updates are given in the sections "Nonlinear Case" (Cooley, 1992) and "Nonlinear Conditions" (Torak, 1993).

The nonlinear steady-state versions of MODFE require the following inputs for defining the iterative-solution method: values for the maximum number of water-table iterations, maximum allowable displacement, and closure tolerance for steady state. The maximum number of water-table iterations is represented by the program variable NITSW. The number of iterations needed to reach an acceptable nonlinear solution varies for each simulation, and is dependent on the number of nonlinear conditions that exist in the aquifer problem, the maximum allowable displacement, and the closure tolerance. Most nonlinear steady-state problems can be solved with fewer than 50 water table iterations.

The maximum allowable displacement, or head change, is represented by the program variable DSMX. Head changes greater than DSMX that are computed during an iteration level are damped (decreased) before they are used to update aquifer thickness and to evaluate nonlinear-boundary conditions. For highly nonlinear problems; that is, simulations involving many nodes that require evaluation of nonlinear conditions, values of DSMX should be selected smaller than about half of the expected head change from the initial to the final conditions. Specification of DSMX in this manner allows updates to nonlinear terms to be made gradually over several water-table iterations, instead of making large changes to nonlinear terms over a few iterations. This latter condition may cause inappropriate updates to the nonlinear terms that can lead to excessive iteration, nonclosure, or closure to an incorrect solution.

The closure tolerance for steady-state is represented in MODFE by the program variable TOLSW, and can be selected so that an acceptable solution to the nonlinear problem is obtained with a minimum number of iterations. Values for TOLSW may be selected initially as an order of magnitude smaller than the accuracy of the observed water levels, and then adjusted to give the desired level of acceptability of flow rates and flow imbalance in the water-balance summary. Usually, the nonlinear solution is accepted when the value for the flow imbalance that is output in the water-balance summary is about five to six orders of magnitude smaller than the largest flow rate. A discussion of mass-balance and error terms is given in the section "Water-Balance Summary and Flow Imbalance" in Torak (1993).

Values for TOLSW may be selected differently than described above if the MICCG method of solution is used. Although the closure tolerance for steady state is independent of the convergence criterion ϵ for the MICCG method (see equations (285) and (289) in Cooley, 1992), the relative values for each criterion may be adjusted to achieve faster convergence than if only TOLSW were adjusted. Selection of values for both closure criteria is discussed in the section "Stopping Criteria," in Cooley (1992).

Other data inputs to the nonlinear steady-state versions of MODFE are similar to the inputs required for linear steady-state versions. These are: a value (1) for the indicator variable ISTD, discussed in the previous section, and nodal values of aquifer thickness (THK) and altitude of the top of the water-table aquifer or the bottom of an overlying confining bed (TOP). Values for the storage coefficient (STR) and specific yield (SY) should be set to zero or left blank. Additional information on these data inputs are given in the section "Input Instructions."

Selecting Stress Periods and Time-Step Sizes

The selection of stress periods and time-step sizes is dependent entirely on the distribution of aquifer stresses over time. A stress period usually defines a time interval over which aquifer stresses and boundary conditions are constant. Stress periods are subdivided into time steps, and solution to the finite-element equations is provided by MODFE for average conditions that exist during the time step. The ability to change stresses and boundary conditions in MODFE for any time step may appear to make stress-periods obsolete. However, changes to particular stresses, such as well-pumping rates, or to boundary conditions that create stress, such as surface-water levels, may occur with a degree of regularity or irregularity, or may define an historic event that requires identification as a stress period, rather than as a change in stress on a time-step basis. For example, ground-water withdrawals may have increased suddenly within a short period of time due to increased demands by population, agriculture, or industry. Thus, one stress period can be established to represent the time prior to the increase in pumping rates, and another stress period can be used to represent the time after the increase was invoked. However, within these stress periods, surface water levels or boundary fluxes also may vary, or a few wells could either cease or begin pumping. It may be determined that these changes either impose minor effects on the aquifer or occur frequently so that they can be represented by time-step variations in stresses or boundary conditions. Thus, for this example, stress periods are established to coincide with major changes in stress on the aquifer.

The use of many stress periods, each containing the same number and size of time steps, may have computational advantages in MODFE over using one stress period having a long series of time steps. If the number and size of the time steps are identical for successive stress periods, then the time-step information from the first stress period that contains identical time-step information as the previous stress period can be used on subsequent stress periods without inputting new time-step data. Also, computer storage is decreased because only the time-step sizes for the first stress period in the succession of identical stress periods are required to be stored. This is accomplished in MODFE by evaluating the indicator variable NTMP at the beginning of the inputs for the stress period (see section "Input Instructions"). A value of zero (0) for NTMP will permit the time-step number and sizes from the current stress period to be used for the following stress period. The savings in computer storage can be large depending on the number of stress periods that can be formed in this manner.

The selection of time-step sizes may have a more theoretical basis than the establishment of stress periods. Of equal importance as spatial discretization of finite-element equations is the discretization of the finite-element equations in time. Although problem dependent, some guidelines can be applied to selecting time step sizes that ensure adequate discretization of the time derivative in equation (1).

Important considerations when selecting time-step sizes are the magnitudes of the initial stresses (or boundary conditions), changes to stresses (or boundary conditions), and the anticipated effects on the aquifer. Large stresses or changes in stress relative to the aquifer's ability to respond may require many small time steps during the initial stages in which the stress is applied in order to adequately represent nonsteady-state flow. Aquifer response may be such that nonsteady-state gradients may be established only a short distance from the stress, and that the aquifer will exhibit nonsteady-state conditions for a long period of time. Small time steps are needed to accurately approximate head changes during nonsteady-state conditions in a manner analogous to the increased discretization by small-area elements that is needed in the vicinity of a pumped well. Time-step sizes can increase from the small sizes that are needed initially to adequately simulate aquifer response to a new or changed stress, to gradually larger time steps as the aquifer response diminishes and steady-state conditions are reached. Accurate results have been obtained by gradually increasing time steps by a factor of 1.1 to 1.5 of the previous value.

The effects of time-step sizes on the solution of hydraulic head and on volumetric flow rates for mass-balance terms can be determined by performing a sensitivity test. Time-step sizes are decreased (or increased) from their initial or previous values and the aquifer problem is simulated again. Values for the volumetric rate of accumulation and total volume of water in aquifer storage, which are computed in the water-balance summary, are noted for each simulation. Simulations are performed until there is no significant change in these values when compared with similar values from the previous simulation. Appropriate time-step sizes for subsequent simulations are determined as the largest time steps that allow maximum values for the volumetric rate and total volume of water in aquifer storage; additional discretization in time (smaller time steps) yield no significant increase in the volumetric rate and total volume of water in aquifer storage.

Proper selection of time-step sizes will provide accurate representation of time-variant terms in nonlinear-flow problems. Solutions to flow problems involving water-table conditions, conversion between confined and unconfined conditions, drying and resaturating parts of the aquifer, and nonlinear head-dependent flux are particularly sensitive to the time-step size. Time-step sizes for nonlinear-flow problems can be smaller than those that are used for linear problems because of the time variation of terms used to form the finite-element equations. Adequate time-step sizes for nonlinear problems can be determined by conducting the sensitivity test described above and by evaluating the flow imbalance which is printed in the water-balance summary. In addition to the criterion described above, suitable time-step sizes are the largest values that allow a flow imbalance to be computed to within the accuracy of computer; that is, about six orders of magnitude smaller than the largest volumetric flow rate in the water-balance summary. Because nonlinear conditions may exist during the entire simulation period, increases to time-step sizes may not be appropriate or may have to be kept small.

Changing Stresses and Boundary Conditions with Time

Stresses, such as point sources and sinks, specified fluxes, and areally distributed fluxes; controlling heads to boundary conditions, such as specified heads; and boundary and external heads to linear and nonlinear head-dependent fluxes, are allowed to vary during a simulation as functions of time. Changes to these terms can be made at any time step of any stress period as determined by the aquifer problem. Depending on the stresses or boundary conditions to be changed, MODFE is structured to contain up to four additional subroutines, and the corresponding Fortran call statements, to perform the related computations and data inputs. In addition, most of the stresses and boundary conditions that are permitted to change with time require two time steps to implement the change (Table 1). Details of these computations are given in the section "Changing Stresses and Boundary Conditions with Time" in Torak (1993). Program structures are given in the section "Program Structures and Lists of Main Programs" in Torak (1993).

Time variance of stresses and boundary conditions are represented in finite-element matrix equations (254) and (257) in Cooley (1992) by the vector B, which is defined by equations (60)–(62) in Cooley (1992). This formulation requires that the average value of the stress or boundary condition be used when forming the matrix equation. Consequently, average values for the changed stress or boundary condition must be computed by the user and input to MODFE for the time step that the change occurs. On the time step following the change, the user must input the new value for the changed stress or boundary condition, as the average value for the new time step is now the changed value. Thus, changes to stresses and boundary conditions take two time steps to invoke.

Changes to stresses and boundary conditions by using the two-time-step procedure described above are demonstrated by the following example. Consider changing the external head, H_B, on a head-dependent (Cauchy-type) boundary from its current value of 100 feet to 109 feet on the following time step of a simulation. The user computes the average value of H_B according to the expression for the average B vector, equation (62) in Cooley (1992), as 106 feet, or, (1/3) × 100 feet + (2/3) × 109 feet. This value (106 feet) is input to MODFE on the first time step in which the change is take effect. On the following time step, the user computes the average value of H_B as 109 feet, (1/3) × 109 feet + (2/3) × 109 feet, and inputs the new value of H_B (109 feet) to MODFE. Subsequent time steps use the value of 109 feet for H_B until another change takes place. If changes to H_B are made on successive time steps, then average values for H_B are computed by the user according to equation (62) in Cooley (1992) and are input on every time step in which a change is to take effect. The last 'new' value for H_B is input on the time step following the last change.

An exception to using two time steps for changing boundary conditions as described above applies to changing values of head at specified-head boundaries and source-layer heads that are used to simulate transient leakage (see Table 1). For these two cases, the average head is computed automatically within MODFE according to equation (62) in Cooley (1992). Thus, the user inputs only the new values for these heads; changes to these boundary conditions are made in MODFE by using one time step.

Changes to point sources and sinks and areally distributed fluxes require the old value to be input along with either the average or the new value when a change is made (Table 1). The old values are needed to adjust the appropriate mass-balance terms, as the known fluxes are not represented by individual program variables at each node.

Each stress or boundary condition that is allowed to change during the simulation has an indicator variable assigned to it. The values for the indicator variables define the time step on which the change is to occur. On the appropriate time step, inputs corresponding to changes in stresses or boundary conditions are read by MODFE. In addition to these inputs, a new value for the indicator variable is input to allow changes on subsequent time steps. If two time steps are required to change a stress or boundary condition, then the indicator variables contain the appropriate time-step numbers that would permit changes to be made on successive time steps. Although it is possible to input initial conditions of stresses or boundary conditions by indicating a change on the first time step of the first stress period (indicator variables set to 1 followed by the appropriate inputs), initial values are input more

Table 1.—Program variables and subroutines used to change stresses and boundary conditions with time

Stress or boundary condition	Number of time steps to implement change	Indicator variable	Old value	New value	Subroutine
Source-bed head for transient leakage	1	NCBCH	--	HRJ	CBCHG
Point sources/sinks	2	NWCH	QOLD	QNEW	COCHG
Areally distributed recharge/discharge	2	NQCH	QOLD	QNEW	COCHG
Source-bed head for steady leakage	2	NHRCH	--	HR(J)	COCHG
Specified-flux boundary	2	NBQCH	--	QNEW	COCHG
Head-dependent (Cauchy-type) boundary	2	NBQCH	-- --	HK(J) HL(J)	COCHG
Specified-head boundary	1	NHCH	--	HB	COCHG
Nonlinear head-dependent (Cauchy-type) boundary	2	NGNCH	-- --	HRK(J) HRL(J)	GNCHG
Controlling head for nonlinear steady leakage	2	NVNCH	--	HS(J)	VNCHG

easily by using the input mechanisms designed for initial conditions (see section "Input Instructions" for descriptions of indicator variables and other inputs) than the subroutines and inputs designed to change these values.

Inputs consisting of the changed values for stresses or controlling heads are made on each time step according to the sequence given in the input instructions. Entries are omitted from the sequence of inputs for a particular time step if the related stress or controlling head is not to be changed. Conversely, multiple inputs of changes to one type of stress or boundary condition may precede entries for other types, if a particular change is made more frequently than others. Details of these inputs are given in the sections "Input Instructions" and "Examples of Model Input."

Data Preparation

All data that are required for simulating a given aquifer problem are prepared for input to MODFE according to the instructions given in the section "Input Instructions." However, the input of hydraulic properties, boundary conditions, and the finite-element mesh to MODFE can be simplified. Hydraulic properties and boundary conditions that are input by element and element side can be grouped by common values into hydraulic-property and boundary-condition zones. Another simplification involves combining the input of node numbers that define elements (element incidences) so that one set of incidences define two triangular elements. The following sections describe how to combine element incidences, establish hydraulic-property and boundary-condition zones, and input values to MODFE.

Combined-Element Incidences

The node numbers that define an element, termed element incidences, can be combined for two contiguous elements for input to MODFE. Combining element incidences simplifies input, decreases computer-storage requirements, and utilizes the efficient programming style of MODFE most effectively. To combine element incidences, the four node numbers that define an element pair (two contiguous elements) are written in counterclockwise order (fig. 30*A*). The element pair is divided into two triangular elements (fig. 30*B*) along the element side defined by the first and third element incidences (nodes 35 and 42 in fig. 30*A*).