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

Chapter A3

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

By Lynn J. Torak

Book 6
MODELING TECHNIQUES

U.S. DEPARTMENT OF THE INTERIOR
BRUCE BABBITT, ***Secretary***

U.S. GEOLOGICAL SURVEY
Dallas L. Peck, *Director*

UNITED STATES GOVERNMENT PRINTING OFFICE: 1993

For sale by U.S. Geological Survey, Map Distribution
Box 25286, MS 306, Federal Center
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PREFACE

The series of manuals on techniques describes procedures for planning and executing specialized work in water-resources investigations. The material is grouped under major subject headings called "Books" and further subdivided into sections and chapters. Section A of Book 6 is on ground-water modeling.

The unit of publication, the chapter, is limited to a narrow field of subject matters. This format allows flexibility in revision and publication as the need arises. Chapters 6A3, 6A4, and 6A5 are on the use of a particular transient finite-element numerical method for two-dimensional, ground-water-flow problems. These Chapters (6A3, 6A4, and 6A5) correspond to reports prepared on the finite-element model given the acronym MODFE and designated as parts 1, 2, and 3, respectively. Part 1 is on "model description and user's manual," part 2 is on "derivation of finite-element equations and comparisons with analytical solutions," and part 3 is on "design philosophy and programming details."

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[1]This manual is a revision of "Measurement of Time of Travel and Dispersion in Streams by Dye Tracing," by E.F. Hubbard, F.A. Kilpatrick, L.A. Martens, and J.F. Wilson, Jr., Book 3, Chapter A9, published in 1982.
[2]Spanish translation also available.

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[1]This manual is a revision of TWRI 5–A3, "Methods of Analysis of Organic Substances in Water," by Donald F. Goerlitz and Eugene Brown, published in 1972.

[2]This manual supersedes TWRI 5–A4, "Methods for collection and analysis of aquatic biological and microbiological samples," edited by P.E. Greeson and others, published in 1977.

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A MODular Finite-Element Model (MODFE) for Areal and Axisymmetric Ground-Water-Flow Problems Part 1: Model Description and User's Manual

By Lynn J. Torak

Abstract

A *MODular*, *Finite-Element* digital-computer program (MODFE) was developed to simulate steady or unsteady-state, two-dimensional or axisymmetric ground-water flow. Geometric- and hydrologic-aquifer characteristics in two spatial dimensions are represented by triangular finite elements and linear basis functions; one-dimensional finite elements and linear basis functions represent time. Finite-element matrix equations are solved by the direct symmetric-Doolittle method or the iterative modified, incomplete-Cholesky, conjugate-gradient method. Physical processes that can be represented by the model include (1) confined flow, unconfined flow (using the Dupuit approximation), or a combination of both; (2) leakage through either rigid or elastic confining beds; (3) specified recharge or discharge at points, along lines, and over areas; (4) flow across specified-flow, specified-head, or head-dependent boundaries; (5) decrease of aquifer thickness to zero under extreme water-table decline and increase of aquifer thickness from zero as the water table rises; and (6) head-dependent fluxes from springs, drainage wells, leakage across riverbeds or confining beds combined with aquifer dewatering, and evapotranspiration.

The report describes procedures for applying MODFE to ground-water-flow problems, simulation capabilities, and data preparation. Guidelines for designing the finite-element mesh and for node numbering and determining band widths are given. Tables are given that reference simulation capabilities to specific versions of MODFE. Examples of data input and model output for different versions of MODFE are provided.

Introduction

This is the first report of a three-part series of reports that documents MODFE, a MODular, Finite-Element, digital-computer program. This report is intended to be a user's manual that describes applications of MODFE for simulating the physical processes associated with two-dimensional and axisymmetric ground-water flow. The development of matrix equations that are solved by MODFE is given in a companion report, Part 2 (Cooley, 1992). Similarly, details of the modular program design are given in Part 3 (Torak, 1993). Simulation capabilities of MODFE include:

- 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.

Elements of the simulation capabilities listed above are described with regard to their representation of hydrologic characteristics of ground-water-flow problems and their implementation in MODFE. Examples are given that show alternate formulations for representing the same hydrologic characteristic, such as leakage to or from a river, and the circumstances under which each form would apply during simulation.

A discussion of design considerations for the finite-element mesh is given to provide important background information to the model user about creating a mesh with the appropriate subdivision (discretization) where needed within the region to be simulated. Methods for recognizing and minimizing errors in the computed solution that are related to the discretization scheme also are provided. Generalized rules are given as guidelines to proper mesh construction for most applications of MODFE.

Several methods of improving the computational efficiency and ease of data input are discussed in this report. These include selecting either a direct or an iterative method to solve the finite-element equations, numbering nodes in the finite-element mesh to ensure efficient use of computer storage and of the direct-solution method, and preparing hydrologic information for data input by zone. Example simulations are used to demonstrate data input and program output, and input instructions are given.

Background

Descriptions of the numerical representation of physical processes and hydrologic features contained in this and the companion reports have evolved over the past 10 years from material presented by the authors in the course "Finite-Element Modeling of Ground-Water Flow," held at the U.S. Geological Survey National Training Center in Denver, Colorado. This report formalizes the course material, which has been revised to incorporate comments and suggestions from attendees of the courses.

Purpose and Scope

This report is a guide to using MODFE for simulating two-dimensional, ground-water-flow problems of varying complexity. Concise descriptions are given for representing hydrologic characteristics of ground-water-flow problems numerically and by the finite-element method used in MODFE. Discussions of simulation capabilities emphasize how the model user would convert real-world, hydrologic conditions into a numerical representation for solution. Details concerning computational aspects of MODFE are not included in this report. In like manner, the model equations also are not developed. These aspects of MODFE are given proper emphasis in companion reports by Cooley (1992) and Torak (1993), so that this report can focus on the hydrologic aspects of applying MODFE to solve ground-water-flow problems. Hence, a user can begin to simulate aquifer problems with MODFE after only a short investment in time spent reading this report.

Governing Equation

MODFE solves the two-dimensional, unsteady-state equation of ground-water flow given by equation (1) in Cooley (1992), for hydraulic head h, subject to the boundary conditions expressed by equations (2) through (5) in Cooley (1992). This equation is restated as

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}+T_{xy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial y}\left(T_{yx}\frac{\partial h}{\partial y}+T_{yy}\frac{\partial h}{\partial y}\right)+R(H-h)+W+P=S\frac{\partial h}{\partial t} \quad (1)$$

where

(x,y)= Cartesian coordinate directions [length],

t= time [time],

h(x,y,t)= hydraulic head in the aquifer [length],

H(x,y,t)= hydraulic head in the source layer [length],

$\begin{bmatrix} T_{xx}(x,y,h,t) & T_{xy}(x,y,h,t) \\ T_{yx}(x,y,h,t) & T_{xy}(x,y,h,t) \end{bmatrix}$ = symmetric transmissivity tensor written in matrix form [length^2/time]

R(x,y,t)= hydraulic conductance (vertical hydraulic conductivity of a confining bed divided by its thickness) [time^{-1}],

S(x,y,t)= storage coefficient [0],

W(x,y,t)= unit areal recharge or discharge rate (positive for recharge) [length/time], and

$P(x,y,h,t)=\sum_{j-1}^{p}\delta(x-\alpha_j)\delta(y-b_j)Q_j=$ Dirac-delta designation for p point sources or sinks, each of strength Q_j [length/time] and located at (a_j,b_j). Q_j is positive for injection.

Both confined (linear) and water-table (nonlinear) conditions are simulated by MODFE and are represented by equation (1). For confined ground-water flow having linear boundary conditions, terms in equation (1) that multiply either hydraulic head, h(x,y,t), or derivatives of head, or terms that represent boundary flows, are not functionally dependent on head and are constant in time. An example is ground-water flow in a confined aquifer having linear boundary conditions, where neither the transmissivity nor storage coefficient are functions of head.

When applied to nonlinear ground-water flow, equation (1) contains terms that are functionally dependent on hydraulic head. For example, in a water-table (unconfined) aquifer, transmissivity is a function of hydraulic conductivity, K, and changing aquifer thickness, b, which is a function of changing hydraulic head. That is, $b = h - z_b$, where z_b is the altitude of the aquifer bottom, and $T = K(h - z_b)$, (see equation (65) of Cooley, 1992). Another example of nonlinear conditions occurs when aquifers convert from confined to unconfined (or from unconfined to confined) conditions during the simulation, where the storage coefficient and transmissivity change with time depending on the value of hydraulic head relative to the base of the overlying confining bed.

Terms accounting for steady vertical leakage, $R(H - h)$ in equation (1), or Cauchy-type boundaries, $\alpha(H_B - h)$ in equation (4), (Cooley, 1992), will cause equation (1) to be nonlinear if R, α, or the head differences change as a function of aquifer head. Typical applications of these nonlinear-leakage functions are given in subsequent sections of the user's manual and involve simulation of rivers, springs or drainage-well discharge, evapotranspiration, and vertical leakage from an overlying confining bed when the aquifer converts from confined to unconfined (or from unconfined to confined) conditions.

Procedure for Applying the MODular Finite-Element Model (MODFE) to Ground-Water-Flow Problems

The procedure for applying MODFE to two-dimensional ground-water-flow problems begins by constructing a finite-element mesh that will accurately represent hydrologic factors such as hydraulic head, aquifer geometry, and boundary conditions within the region to be simulated. The following section provides guidelines for mesh construction, and gives examples of how these hydrologic aspects can be represented by subdivision, or discretized, with triangular elements, element sides, and (or) element intersections (nodes) in a finite-element mesh.

After a suitable finite-element mesh is constructed, the next step is to number the nodes in a manner that minimizes computer storage and execution time; this increases the computational efficiency of MODFE. Techniques are discussed for minimizing the maximum difference between node numbers in any element (termed the matrix bandwidth) and for minimizing the maximum number of element connections to any node (termed the condensed semibandwidth), two factors related to mesh design and node numbering that affect computational efficiency. Examples are given that show node-numbering schemes and their effects on computer storage, and how to eliminate excessive element connections to any node by redesigning parts of the mesh. Although these discussions follow the section on mesh design, they provide valuable information that a user should consider during construction of a finite-element mesh.

The next step in applying MODFE to solve a ground-water-flow problem is to select a solution method to the finite-element matrix equations that are formed by the program. Information is provided about the direct (symmetric-Doolittle) method of triangular decomposition and about the iterative, modified Cholesky, conjugate-gradient method so that the user can decide which method will better suit the aquifer problem to be solved. Like the previous considerations for mesh design and node numbering, selection of either solution method is a matter of computational efficiency rather than numerical accuracy.

Design Considerations for the Finite-Element Mesh

This section describes how to design a finite-element mesh to account for the pertinent hydrologic factors that are present in ground-water-flow problems that can be solved by using MODFE. The accurate representation of hydrologic factors that affect ground-water flow in an aquifer depends partly on accurate approximations to the ground-water-flow equations by the finite-element method, as discussed in Cooley (1992), and partly on the design of the finite-element mesh. Factors such as locations of flow boundaries and wells, aquifer geometry, distribution of hydrologic properties, and shape of the anticipated potentiometric surface, all influence mesh design. These factors are discussed relative to representing an aquifer region with triangular elements, element sides, and nodes, which together comprise a finite-element mesh.

Parts of this section contain descriptions of concepts of the finite-element method that were developed in Cooley (1992) and that influence the design of a finite-element mesh. Descriptions are given about the manner in which the finite-element method allows hydraulic head and hydrologic properties to vary within the area to be simulated, and how these variations can be represented accurately by the mesh design. A discussion is presented about errors in the computed heads over space and time that are caused by a poorly designed mesh (termed discretization errors), that is, a mesh that does not adequately account for these concepts, and guidelines are given so that a user can test for and minimize the effects of these errors.

Concepts of the Finite-Element Method

Before discussing how a finite-element mesh can be constructed to represent the hydrologic factors that influence ground-water flow in an aquifer, some basic concepts about the finite-element method used in the development of MODFE are described as they relate to mesh design. As stated in Cooley (1992), a basic concept of the finite-element method is that a complex flow region can be subdivided into a network of subregions, called elements, each having a simple shape. The element shapes used by MODFE are triangles, which can approximate curved boundaries of the flow region by careful placement of element sides. Elements are constructed over the region so that the sides of one element coincide completely with the sides of adjacent elements. Elements are joined along common sides and at vertices, which are called nodes, and nodes are located only at element vertices (fig. 1*A*). Hydraulic head is computed at the node points by MODFE. The network of triangles over the flow region is called a finite-element mesh.

The concept of variation in hydraulic head within an element is discussed briefly as it relates to mesh design. Hydraulic head is approximated at any point, (x,y), within an element, e, by a simple algebraic equation, or function, for a plane, $\hat{h} = A^e + B^e x + C^e y$ (equation (6) in Cooley, 1992). Values for the function, $\hat{h}$, are defined at the node (fig. 1*B*). This allows coefficients A^e, B^e, and C^e to be determined from nodal values of $\hat{h}$. The relations of A^e, B^e, and C^e to $\hat{h}$ permits $\hat{h}$ to vary linearly within an element, and solution of h within an element is known, given the values of $\hat{h}$ at the nodes. (See development of equations (6) through (10) in Cooley (1992), for details.)

Each element in the finite-element mesh represents a plane of the function $\hat{h}$, which represents hydraulic head. The orientation of the plane in space depends on the values of $\hat{h}$ at the nodes (fig. 1*B*). On an element side, $\hat{h}$ is a linear function of head at the nodes that define the side; the head at the third node in the element is not used to define $\hat{h}$ along this side. Thus, sides of adjacent elements have the same orientation in space so that the mesh forms a network of piecewise continuous planes of $\hat{h}$ within the aquifer region (fig. 1*C*).

Shape of the Anticipated Potentiometric Surface

An important consideration in the design of the finite-element mesh is the shape of the anticipated solution of hydraulic head, or, of the potentiometric surface, within the aquifer region. The network of triangular planes that comprises a finite-element mesh has the versatility to represent changes in hydraulic heads and in gradients that occur within the aquifer region during simulation, provided that these changes are anticipated and are accommodated by the mesh design. In designing a finite-element mesh, the user should identify any anticipated stresses on the flow system and attempt to understand how these stresses will affect the simulated potentiometric surface. For example, initiating or discontinuing well pumpage, or changing existing well-pumping rates or boundary flows, can cause changes in hydraulic gradients over short distances within the aquifer region. Lateral discontinuities in aquifer properties, caused by abrupt changes in aquifer thickness or lithology, can cause hydraulic gradients to change as the discontinuities are crossed.

For a finite-element mesh to represent a potentiometric surface accurately, the network of triangular planes should be able to approximate curved surfaces well. As discussed in the previous section, each element is a plane that represents part of the potentiometric surface. The orientation of each plane is defined by the values of head at the three nodes describing the element (fig. 1*B*,*C*). On a highly curved potentiometric surface, such as near a pumped well or wells, many elements of small area are required to represent the changing orientation (hydraulic gradients) of the surface (fig. 2*A*). Conversely, where the potentiometric surface is nearly flat and contains only slight changes in hydraulic gradient, such as in an undeveloped, relatively homogeneous aquifer, elements of larger area than those used near a pumped well would be sufficient for representing the surface (fig. 2*B*). However, if the effects of a well field or similar stress is to be simulated on the undeveloped aquifer, then small elements should be used in regions where the anticipated stress is to be applied so that changing hydraulic gradients can be represented adequately by the mesh during simulation of the anticipated stress.

The steepness of hydraulic gradients in the anticipated solution is not as important a design consideration as the change in gradients with distance. Hydraulic gradients that are constant or that do not vary appreciably within the aquifer region, regardless of slope, indicate a relatively noncurving potentiometric surface that can be approximated accurately by using a few large elements. However, where a transition between steep and gentle gradients occurs, or where a transition is anticipated, a curved potentiometric surface can be created. These areas might require subdivision by using many small elements (fig. 3).

Aquifer Geometry and Hydrologic Boundaries

Curved or irregularly shaped aquifer geometry and hydrologic boundaries influence the potentiometric surface within an aquifer region, and therefore, influence the design of the finite-element mesh. Locations of these features can be approximated nearly exactly in a mesh by using element sides, as shown in figure 4. Element sides that define the irregular geometry of aquifer-region boundaries can be used to represent specified-head (Dirichlet), specified-flow (Neumann), or mixed (Cauchy-type) conditions. The location of zone boundaries for hydraulic properties can be represented accurately with element sides (fig. 4).

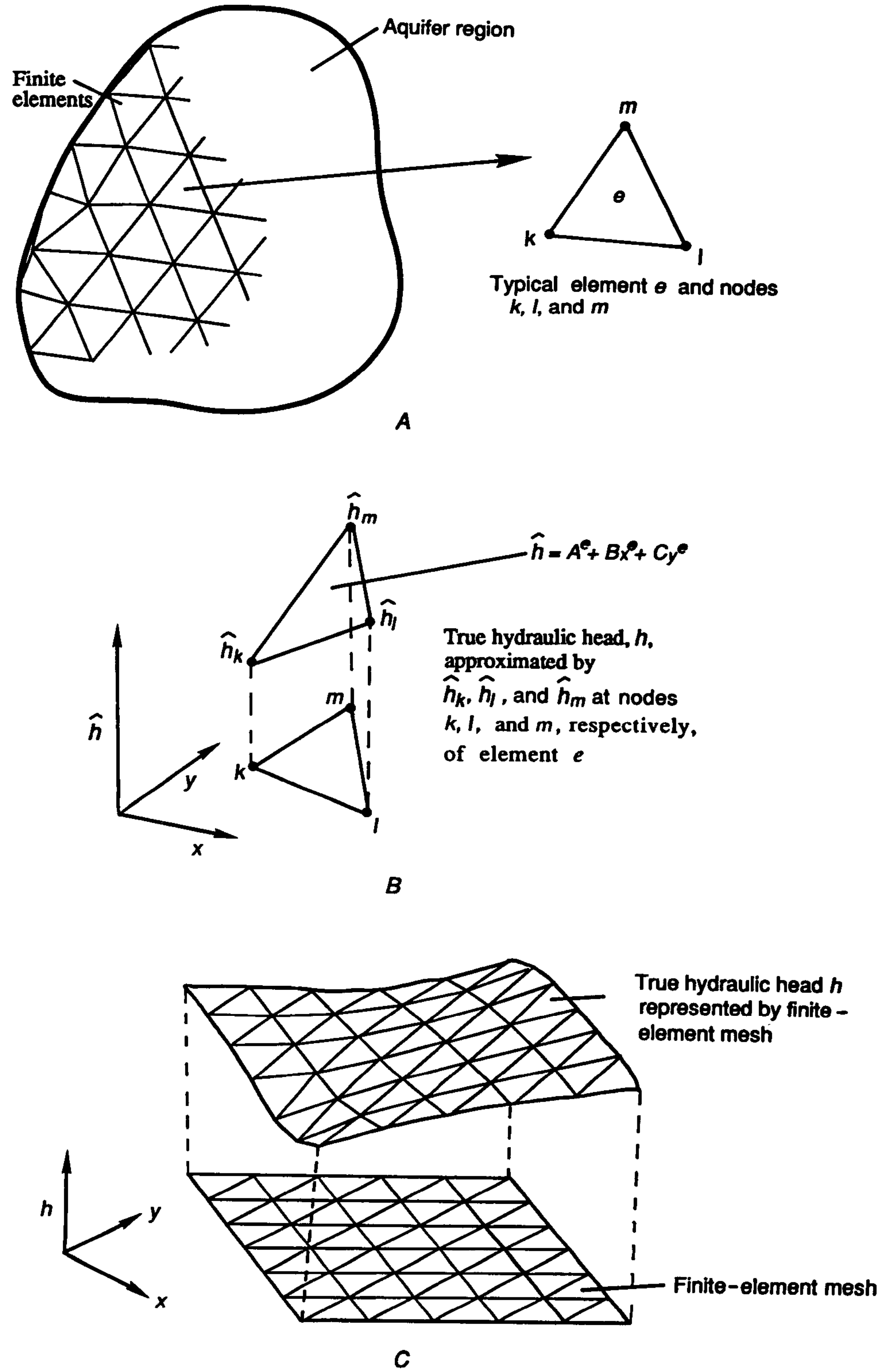

Figure 1.—Diagrams showing (*A*) aquifer region partially subdivided by finite elements and typical element *e*; (*B*) finite-element representation of hydraulic head $\hat{h}$; and (*C*) finite-element mesh configuration for approximating true hydraulic head *h*.

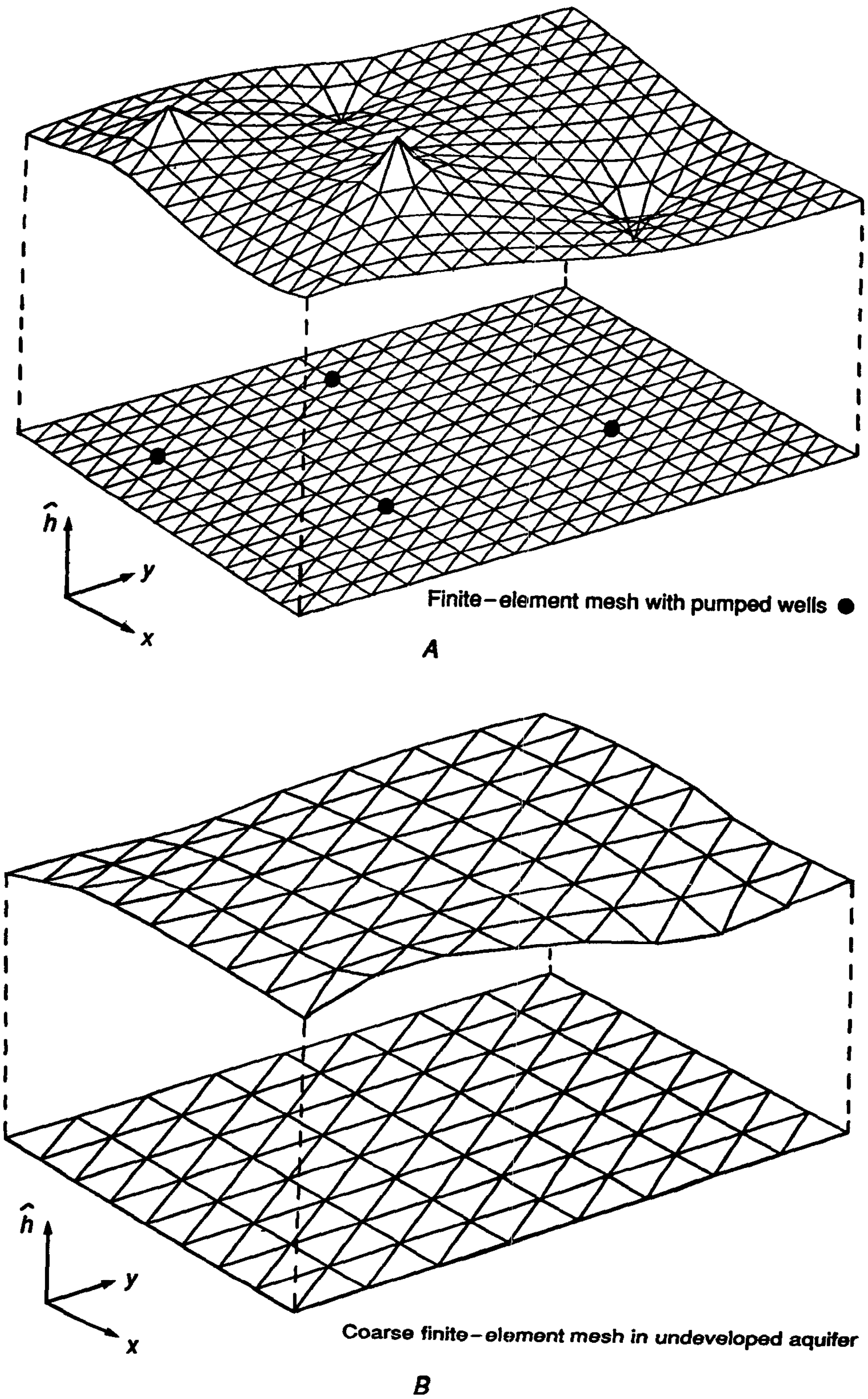

Figure 2.—Representation of potentiometric surface by finite elements (*A*) near pumped wells; and (*B*) in an undeveloped aquifer.

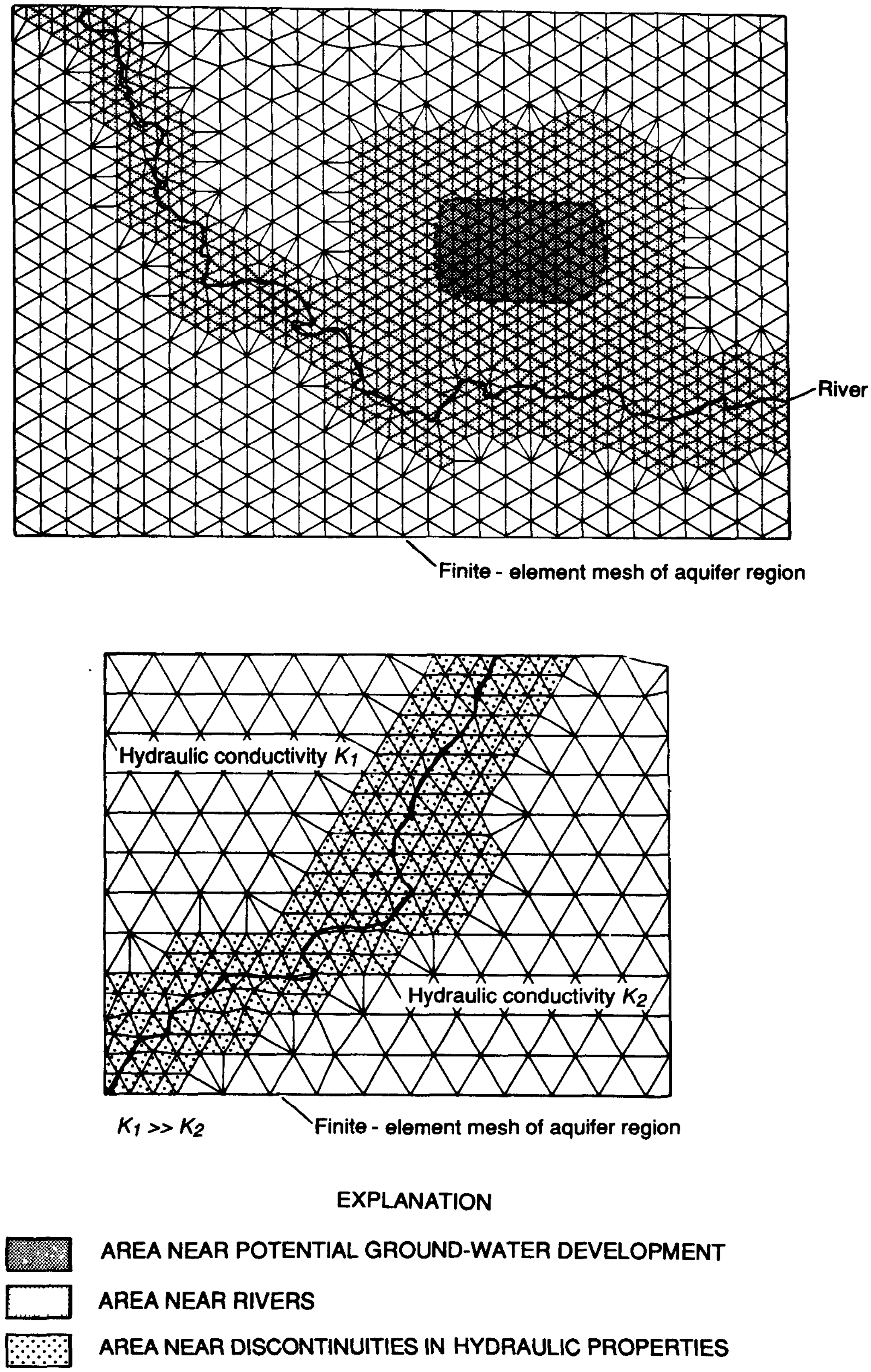

Figure 3.—Examples of additional subdivision by finite elements in areas of changing hydraulic gradient with distance.

As stated in the previous section, changes in hydraulic properties represent discontinuities in the ground-water-flow system that may cause changes in hydraulic gradients within the aquifer region. Hence, accurate location of hydraulic-property zones is necessary to simulate ground-water flow accurately. Rivers also can be represented by element sides in the same manner as hydraulic-property zones. Impermeable (no-flow) boundaries within the aquifer region can be simulated as either a "hole" in the finite-element mesh (fig. 4), or as a zone of elements that contain hydraulic properties of zero. (A discussion of hydraulic-property zones is given in a later section.)

The irregularly shaped and curved contacts between hydrologic units in cross section can be represented easily by element sides. The flexibility in mesh design is particularly useful for representing contacts between units that are folded or arcuate shaped, or where hydrologic boundaries create irregular aquifer geometry (fig 5*A*). Aquifer "pinchouts" or facies changes are represented by positioning element sides along the contacts between units (fig. 5*B*). Combining this aspect of mesh design with the capability to change directions of anisotropy within the aquifer region enables simulation of a wide range of aquifer problems in cross section by using MODFE. (See section "Cross Sections.")

Points of Known Hydraulic Head and Stress

Locations within the aquifer region where stresses and hydraulic heads are known can affect the design of the finite-element mesh. Points of known hydraulic head or stress, such as observation or pumped wells, springs, and drains can be positioned exactly in the finite-element mesh by placing nodes at their locations (fig. 2*A*). The mesh is then constructed with these nodes used as vertices for some of the triangular elements. Other design considerations for the finite-element mesh require that additional nodes and elements be used in order to obtain an accurate approximation of the true potentiometric surface.

Comparison of computed heads with measured values can be made easily from the point (nodal) solutions of hydraulic head that are provided by MODFE. Because the computed head at a node approximates a point on the true potentiometric surface, the computed values can be compared directly with measured water levels (or an analytical solution, as in Cooley, 1992), provided the nodes are located at the points of observation. However, if the nodal locations and the measurements do not coincide, then the expression for the approximate solution of head, $\hat{h}$, given by equation (6) of Cooley (1992), can be used to compute hydraulic head at any (x,y) location within an element. This equation uses nodal coordinates and values of head and coordinates of the measurement to compute the head at the specific location.

General Construction Rules

Some general rules are given as a guide to ensure proper construction of the finite-element mesh. Several design considerations have been mentioned in previous sections, and many different triangular-element shapes are permitted by the finite-element method. However, not all element shapes are acceptable for representing hydrologic conditions in an aquifer region. Adherence to the following rules will enable construction of a mesh that addresses the design considerations and has the ability to provide a numerical solution that closely approximates observed conditions. Some construction rules may not require strict adherence, and in some cases, might be inappropriate or inapplicable given the nature of the aquifer problem. Other rules, if violated, may lead to errors in the numerical solution, termed discretization errors. These errors are described briefly after the associated rule, and a reference is given for the interested reader who wishes to pursue a more detailed discussion. Identification of discretization errors and methods for evaluating and minimizing them are discussed in the following section.

— Subdivide the aquifer region as much as possible by using a regular triangular mesh consisting of uniformly sized equilateral triangles (fig. 4). However, other design considerations within the aquifer region, such as discontinuities in hydraulic properties, aquifer geometry, or hydrologic boundaries, may take precedence over strict adherence to this construction rule. Equilateral triangles provide the most accurate representation of hydrologic conditions by minimizing the error associated with approximating hydraulic head with the finite-element method. For a regular triangular mesh, the error of approximation is proportional to the square of the length of an element side. For a mesh consisting of irregular element shapes, the approximation error is proportional to the square of the maximum length of the element sides (Strang and Fix, 1973, chs. 1 and 2).

— Avoid construction of thin, needle-like elements (fig. 6*A*), as these "degenerate" triangles can either affect the numerical stability of the finite-element method (Strang and Fix, 1973, ch. 3), or introduce errors into the approximation of hydraulic head within an element. Although no limitations on the thinness of an element was found in the literature, Strang and Fix (1973, p. 139) indicated that angles as small as 22.5 degrees did not pose a problem with the finite-element method. My experience with mesh design indicates that angles between 30 and 90 degrees are sufficient for subdividing an aquifer region with finite elements.

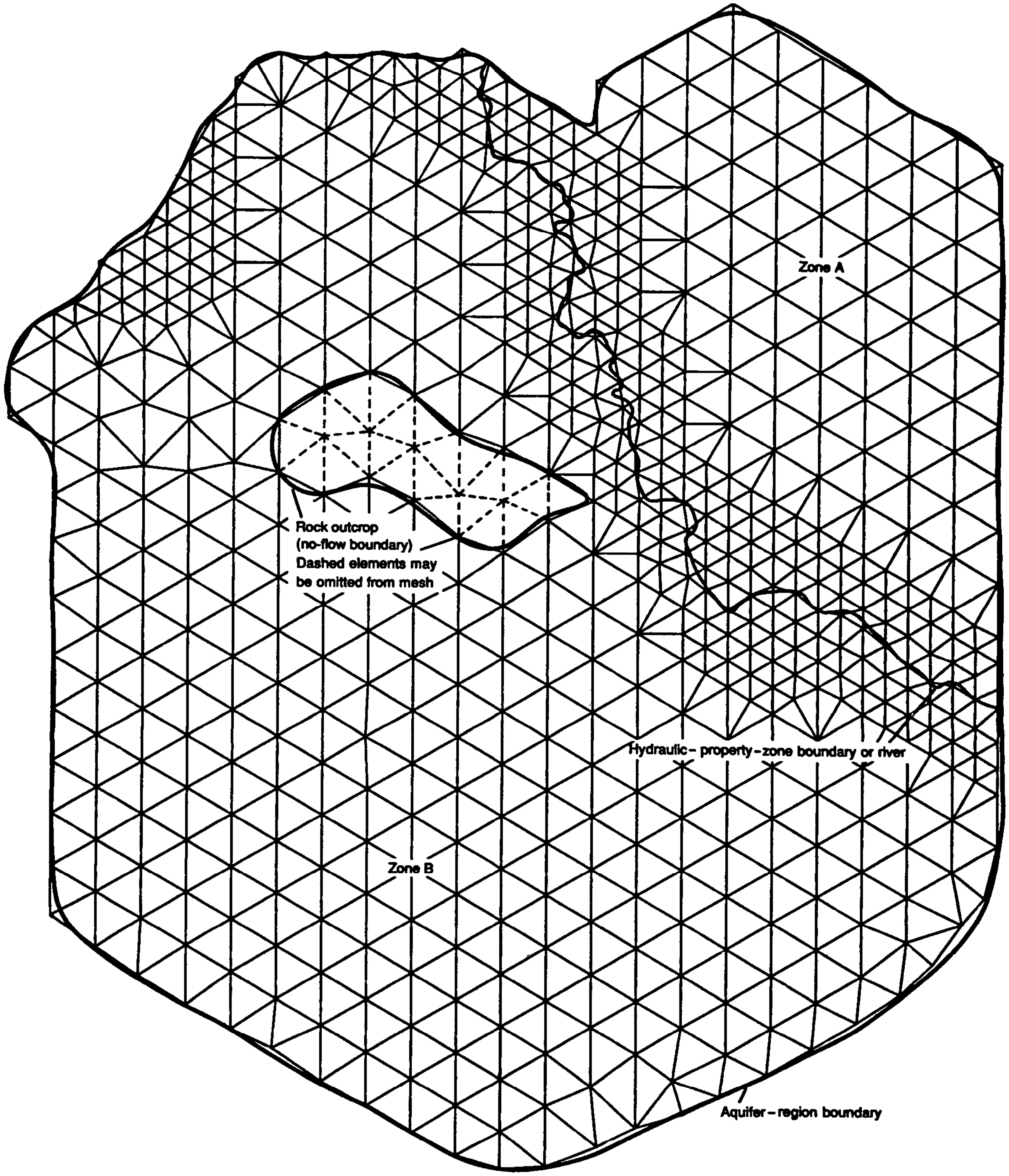

Figure 4.—Approximation by finite elements of curved aquifer geometry and hydraulic-property boundaries.

Smaller angles could be used for specialized problems, such as axisymmetric flow to a well. (See section "Comparisons of Numerical Results with Analytical Solutions," in Cooley, 1992.)

– The sum of two angles created by a side that is common to two elements cannot exceed 180 degrees (fig. 6*B*). Violation of this construction rule results in at least one obtuse angle being created by the side that is shared by the two elements. The existence of obtuse angles in the mesh can be determined by inspection, if the mesh is small, or by a computer program that uses the nodal coordinates as input.

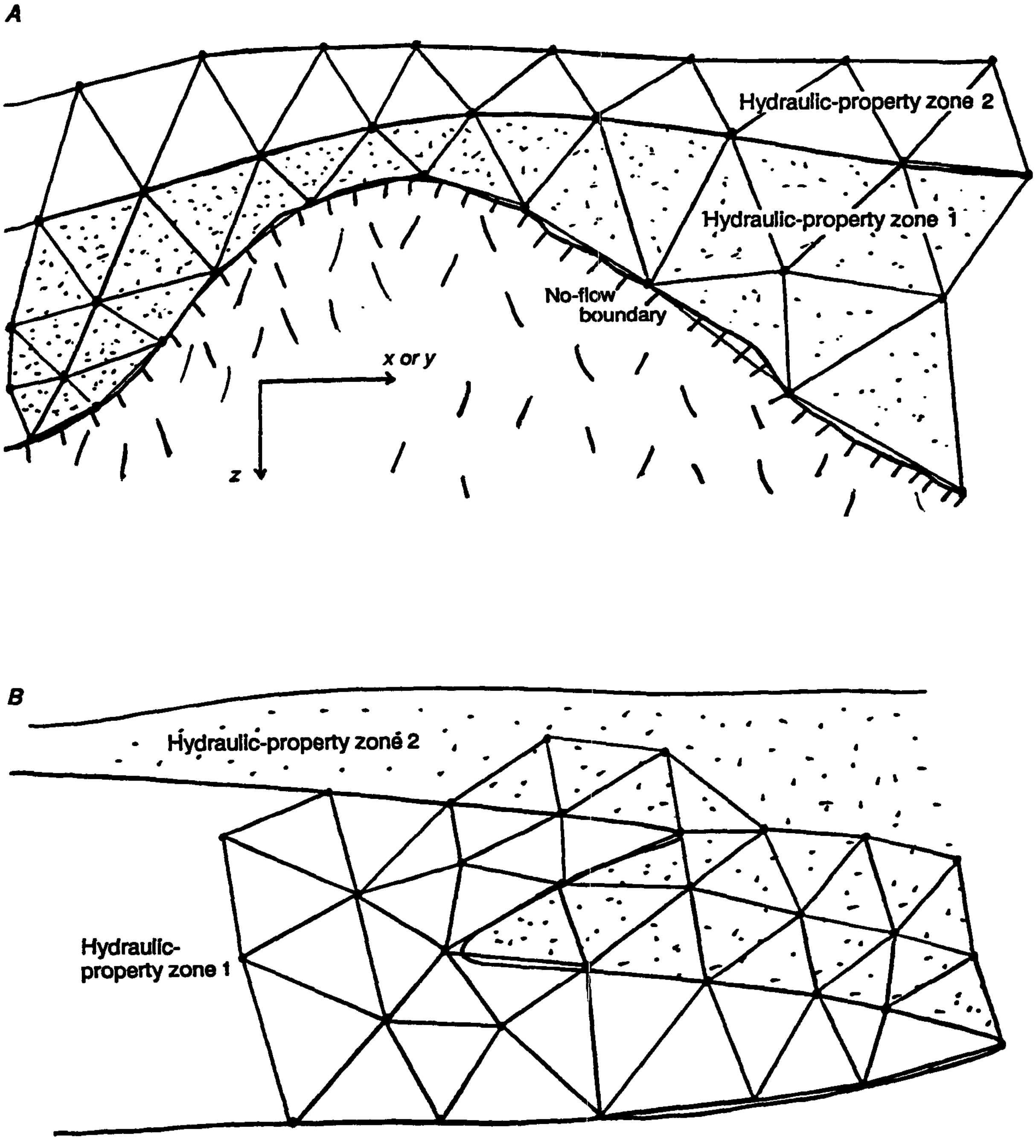

Figure 5.—Representation by finite elements of hydraulic-property zones in cross section (*A*) near arcuate boundaries; and (*B*) along facies changes.

Adherence to this rule ensures diagonal dominance of transmissivity (or hydraulic conductivity) terms in the coefficient matrix G of equation (49) in Cooley (1992). That is, all off-diagonal transmissivity (or hydraulic conductivity) terms in the coefficient matrix are negative, and all main diagonals are positive. This guarantees a non-negative inverse matrix of G, a desirable condition for numerical solution. Because the inverse matrix and the coordinate functions N of equation (9) in Cooley (1992) are non-negative, the finite-element representation of hydraulic head obeys the same physical laws as the true hydraulic head. That is, heads will decrease (increase) when a negative (positive) stress is applied. (See Strang and Fix, 1973, p. 78).

— Incorporate as much aquifer-problem geometry into the finite-element mesh as possible. Curved hydro-

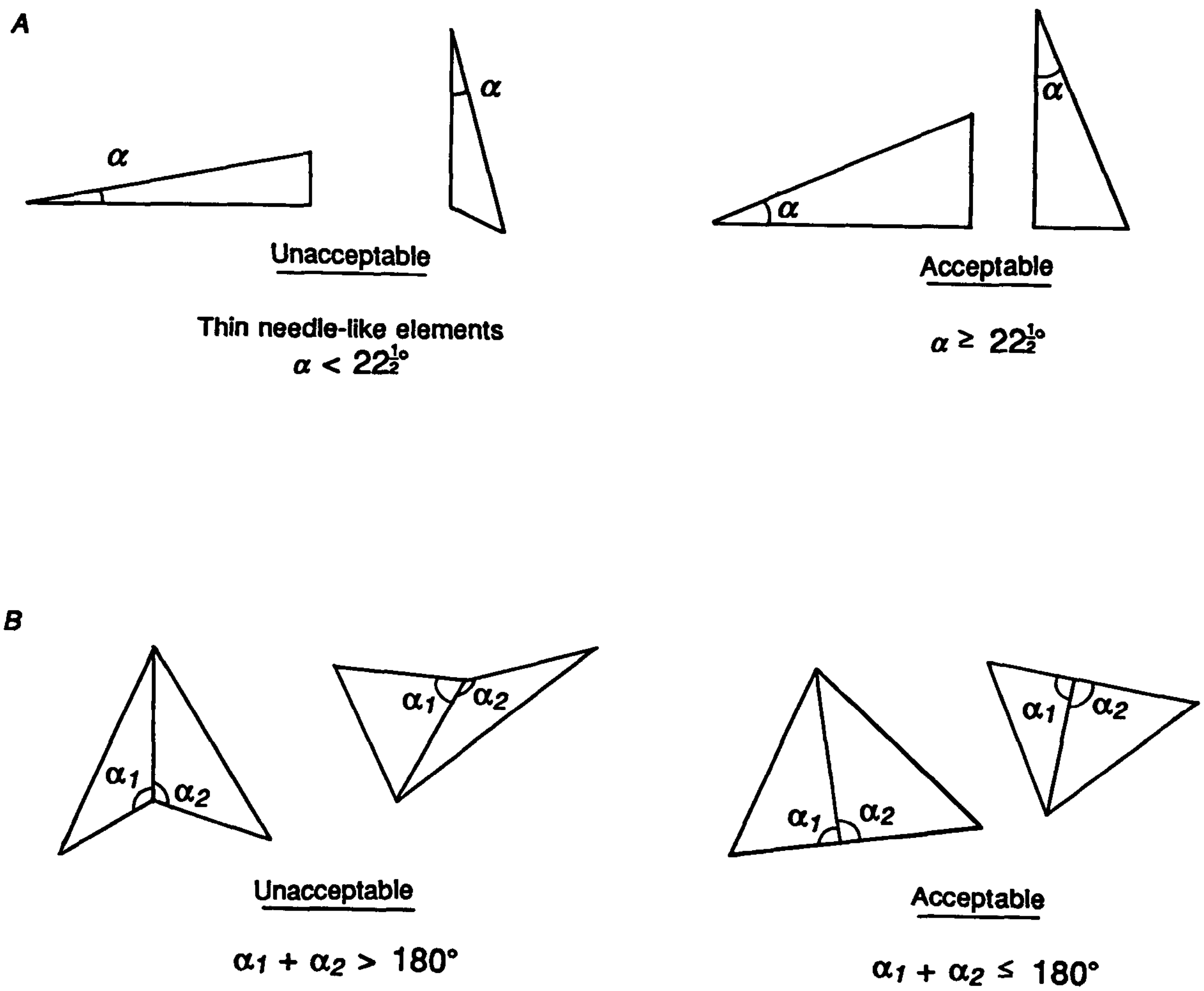

Figure 6.—Acceptable and unacceptable element shapes.

logic boundaries are represented easily by locating nodes on the boundaries (fig. 4). Symmetry in the anticipated solution of hydraulic head requires a corresponding symmetry in the design of the mesh, such as around cones of depression near pumped wells or other stresses (fig. 2).

— Locate points of observation and hydrologic features that are pertinent to an aquifer problem as exactly as possible by using nodes or element sides. Water-level measurements, stresses, and boundary conditions can be represented within the finite-element mesh either as nodes or element sides, allowing for direct comparison of measured values for hydraulic head and flux with the computed solution. However, if nodes cannot represent the location of a water-level measurement exactly, then the value at that location can be determined from values at the surrounding nodes, as described in the section "Points of Known Hydraulic Head and Stress."

— Nodes can be positioned only at vertices of triangular elements.

— Design the mesh so that the number of element sides that connect to any node is fairly uniform throughout the mesh. This construction rule is related more to effective use of computer storage and computation time by MODFE than to the ability of the mesh to represent true hydrologic conditions. This design criterion influences the value of the condensed-matrix bandwidth, which is discussed in the following section.

For most aquifer problems in areal dimensions, a regular triangular mesh can be either drawn by hand or generated by computer to cover the extent of the aquifer region of interest (fig. 4). If additional discretization is needed within the simulated region, then midpoints of element sides can be connected to create four equilateral triangles from each original triangle (fig. 7*A*, dashed lines). The additional nodes, which appear on the midsides of elements that were not subdivided, are then linked by an element side to the

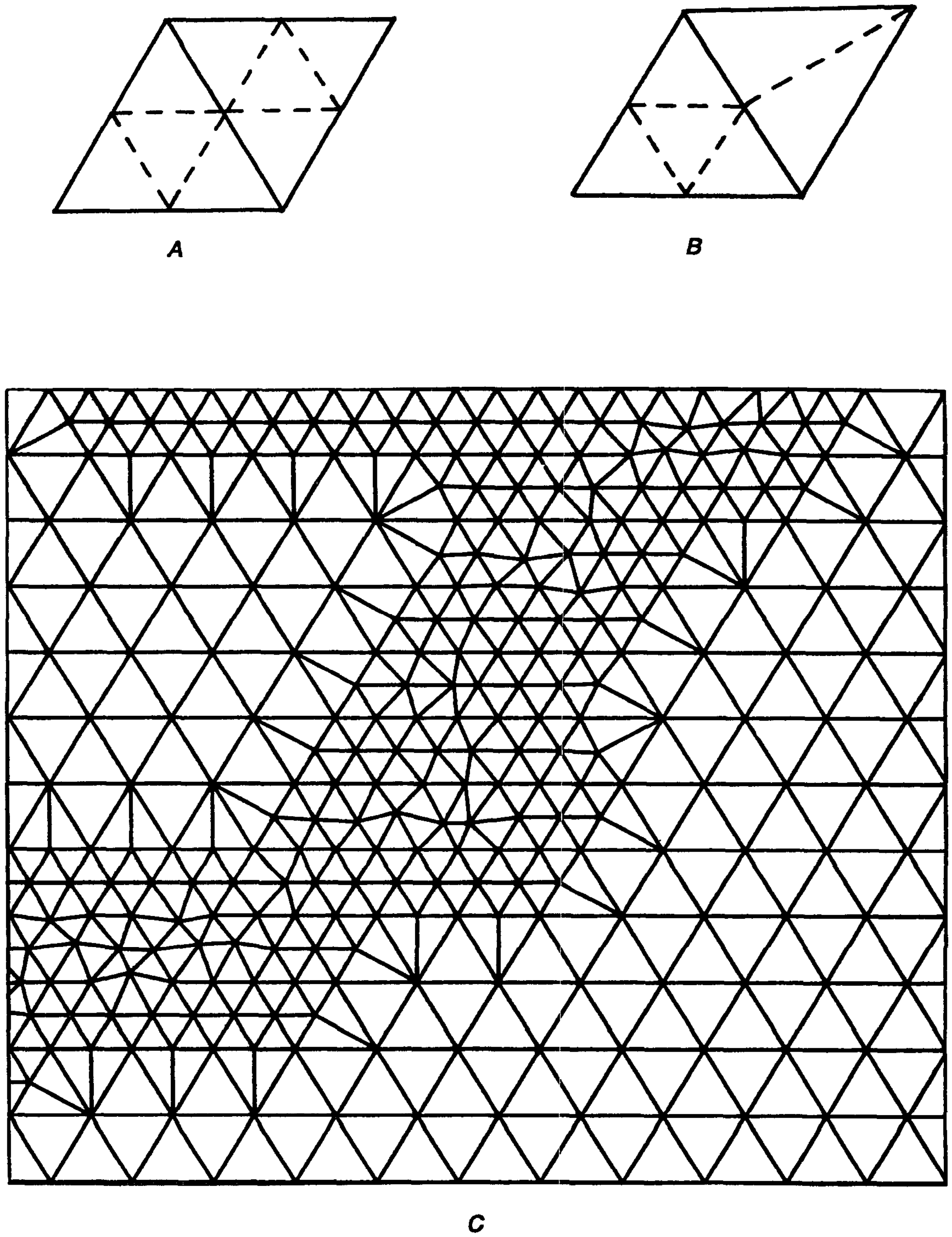

Figure 7.—Subdivision of elements by (*A*) connecting midpoints of element sides and (*B*) connecting midpoint to a vertex. (*C*) Finite-element mesh containing element subdivision.

opposite vertex of the larger element (fig. 7*B*). Subdivision of the formerly unchanged element in this manner creates two elements that are 30–60–90-degree triangles. These concepts of element subdivision are demonstrated in figure 7*C* where the coarse mesh is finely discretized near a river. Note that nodal locations along the river have been moved from the positions that resulted from the element subdivision. By carefully adjusting nodal locations, all angles in the mesh can range from 30 to 90 degrees.

For axisymmetric-cylindrical (radial) flow, the mesh can be designed according to the examples given in the section "Axisymmetric Flow", or according to the mesh used in the radial-flow problems given in Cooley (1992). Depending on aquifer geometry and subsurface lithology, a regular triangular mesh also can be used to discretize the aquifer region in cross section or in axisymmetric flow. However, care must be taken when designing a mesh in axisymmetric coordinates to ensure that the symmetry of the flow problem is represented by the mesh. (See section "Axisymmetric Flow.")

Identifying Discretization Error

The ability of the subdivision (discretization) scheme to accurately approximate the true hydrologic response to stress on the ground-water system is the ultimate test of adequacy in the design of the finite-element mesh. Aside from errors in the characterization of hydrologic properties and in the measurements used to check model validity, discretization error can undermine the computed solution and prevail throughout the study if it is undetected and not corrected. Discretization error may be manifested by the inability of the mesh to represent changing hydraulic gradients in the vicinity of a pumped well or discontinuity in hydrologic properties. Violation of certain mesh-construction rules, described in the previous section, could cause less-than-adequate approximations of hydraulic head within elements. In some cases, discretization error may be subtle, and the user may attempt unsuspectingly to compensate for these by adjusting hydrologic properties during the calibration process or by questioning the accuracy of measurements. In other cases, discretization errors may not be so subtle. In either case, the user must attempt to identify and minimize discretization error during the initial stages of mesh construction.

The process of identifying discretization error in a finite-element mesh is straightforward: the user tests whether refinement of the mesh creates acceptable or unacceptable changes in the computed solution. Mesh refinement involves changing element sizes or shapes, or both, and testing requires determining the effects of these changes on the simulation results. This test can be performed either on part of the aquifer region or on a small, prototype area that contains hydrologic properties and stresses that are characteristic of the aquifer region and the problem. Results of identical simulations that use different finite-element meshes can be compared to determine if the mesh refinements improved the computed solution. For example, if ground-water pumping was simulated under transient conditions, then the computed potentiometric surfaces resulting from fine and coarse discretizations are compared. The mesh that provided improved definition of the potentiometric surface, usually the finer mesh, is preferred over the other mesh. The mesh that provided a more acceptable solution is then further discretized and the simulation is repeated. Testing is concluded when additional mesh refinement does not improve the solution.

Discretization error that is associated with the shape of the finite elements can be identified by inspecting the mesh, if it is small, or by using a computer program to check angles between element sides. A test simulation can be performed after reconstructing part of the mesh that is suspect. Parts of the mesh that contain thin elements or elements that have obtuse angles can be reconstructed to eliminate these occurrences. The simulation is performed with the reconstructed mesh and the results are compared with the previous simulation. A brief discussion of the effects of obtuse angles and thin elements on the finite-element representation of hydraulic head is given in the previous section.

Node Numbering and Determining Bandwidth

After constructing the finite-element mesh, nodes are numbered so that data can be entered. Although node numbering can be arbitrary, certain numbering conventions will improve the computational efficiency of MODFE. For example, by minimizing differences between node numbers in any element, terms used to form coefficients for the finite-element matrix equation (254) in Cooley (1992) will be stored as close together as possible in the computer program, allowing computations to be performed efficiently. The maximum difference between node numbers in an element that does not contain a specified-head node is used to allocate computer storage for the direct-solution method. In a patch of elements, the maximum number of connections from the node in the center of the patch to higher node numbers will determine the computer-storage requirements for each node and the number of storage locations that are overwritten by the iterative, conjugate-gradient method of solution. Allocation of computer storage and execution time is discussed in Torak (1993). Guidelines are given below that will permit a node numbering scheme to be developed that utilizes the computer-storage and computational attributes of MODFE effectively.

Techniques to Enhance Computational Efficiency

Numbering nodes to enhance the computational efficiency of MODFE is related directly to minimizing the reduced-matrix bandwidth and indirectly to minimizing the condensed-matrix bandwidth. The effects

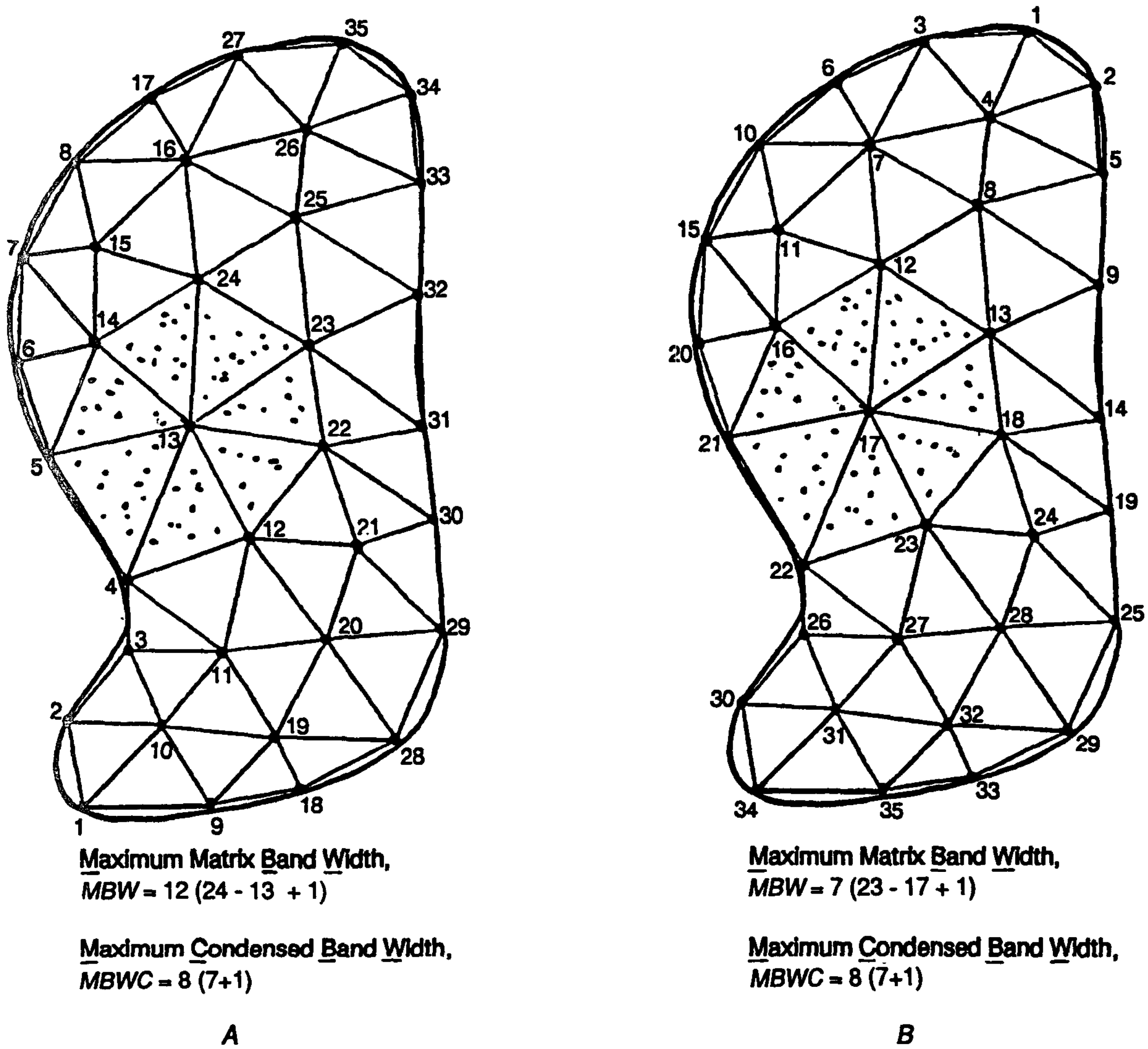

Figure 8.—Effect of node numbering on bandwidth for two identical finite-element meshes (*A*) and (*B*).

of node numbering on both bandwidth determinations are discussed here, and guidelines for bandwidth reduction are given. Definitions for the reduced matrix, condensed matrix, and bandwidths, are given in the following section for reference. In addition, the user can consult the appropriate sections of Cooley (1992) and Torak (1993) for a more detailed description of these terms.

The maximum difference between node numbers in any element and the reduced-matrix bandwidth usually can be minimized by numbering nodes along the shorter direction of the finite-element mesh. For example, given two identical meshes (fig. 8), the mesh that is numbered in the longer direction (fig. 8A) yields a maximum difference between node numbers of 11 (24–13) and a reduced-matrix bandwidth of 12. The mesh that is numbered in the shorter direction (fig. 8*B*) yields a maximum difference between node numbers of 6 (23–17) and a reduced-matrix bandwidth of 7. The reduced-matrix bandwidth is expressed in figure 8 and in MODFE as the program variable MBW. A specific definition of the reduced-matrix bandwidth is given in the following section.

The condensed-matrix bandwidth can be determined by inspecting the finite-element mesh and obtaining the maximum number of nodal connections to any node. Specifically, the condensed-matrix bandwidth is the maximum number of connections to higher-numbered nodes from the node in the center of a patch of elements, plus one. An approximation of the condensed-matrix bandwidth is obtained by counting element sides that are connected to a node in the center of a patch of elements and adding one to this sum. Usually, the value of the condensed-matrix bandwidth is influenced more by mesh design than by node numbering. However, the following example demonstrates that node numbering could be equally important as mesh design in minimizing the condensed-matrix bandwidth.

Consider the patch of elements corresponding either to node 13 in figure 8*A* or to node 17 in figure 8*B*. Although these nodes connect to seven other nodes in the patch of elements, the condensed-matrix bandwidth is determined to be five, as only four of the seven nodes have a higher node number than either 13 or 17, respectively. The condensed-matrix bandwidth is expressed in figure 8 and in MODFE as the program variable MBWC.

The condensed-matrix bandwidth usually is not affected by the size of the finite-element mesh. For regular triangular meshes, the condensed-matrix bandwidth may have a uniform value over the mesh, and the maximum value of MBWC may be determined easily by visual inspection. Irregular meshes make the determination of MBWC difficult; thus, care should be taken in the design of the mesh to avoid excessive element connections to a node.

Definitions

Reduced Matrix—The matrix of coefficients to finite-element matrix equation (254) in Cooley (1992), that results from eliminating equations corresponding to specified-head nodes. This elimination decreases the order of the matrix equation.

Reduced-Matrix Bandwidth—The maximum number of columns between and including the first and last nonzero entries in a row of the reduced matrix. The reduced-matrix bandwidth is estimated as the maximum difference between node numbers in any element that does not contain a specified-head node, plus one. The actual value of the reduced-matrix bandwidth is computed in MODFE by using index numbers to nodes (see sections "Reduced Matrix A" and "Reordering Finite-Element Equations for Solution" in Torak, 1993). It is used in MODFE to expand the condensed matrix prior to solution by the direct-solution method and to allocate computer storage (see section "Allocation of Computer Storage and Processing Time" in Torak, 1993).

Condensed (or Transformed) Matrix—A matrix consisting of the nonzero entries to the right of and including the main diagonals of the reduced matrix. The first column of the condensed matrix stores the main diagonal of the reduced matrix. Off diagonals of the reduced matrix are stored in subsequent columns to the right of the first column (main diagonal of the reduced matrix). This transformation uses the symmetry of the reduced matrix to decrease computer storage and increase the computational efficiency of MODFE.

Condensed-Matrix Bandwidth—The maximum number of nonzero terms across a row of the condensed matrix, determined from the finite-element mesh as the maximum number of higher-numbered nodes that connect to the node in the center of a patch of elements, plus one.

Solution Methods

Two methods for solving finite-element matrix equation (254) in Cooley (1992), are available in MODFE: a direct, symmetric-Doolittle method of triangular decomposition and an iterative, modified, incomplete-Cholesky, conjugate-gradient method (MICCG). Both methods are capable of providing numerical solutions that are limited only by the numerical precision of the computer, thus, each method should be considered equally plausible for the solution of a given matrix problem. The solution methods are interchangeable by replacing the set of subroutines and Fortran call statements pertaining to one method by the set pertaining to the other. Details of replacing solution methods are given in the section "Structure Diagrams for the Main Programs of MODFE", in Torak (1993).

Guidelines for selecting one solution method over the other are based mostly on computational efficiency, that is, the computer storage and time required for completing a simulation. The direct method can be used efficiently on aquifer problems containing a maximum of about 120 to 200 nodes. This limitation is only approximate, as the computational efficiency of the direct method (and the iterative method) is affected by the matrix bandwidths, described in the previous section. Thus, by minimizing the bandwidths, the efficiency of the solution methods is increased.

Both methods can be used to solve linear- or nonlinear-aquifer problems under steady-state or transient conditions. However, as explained in the section "Stopping Criteria" in Cooley (1992), the MICCG method may be more efficient than the direct method for solving nonlinear problems. Other guidelines and descriptions of data inputs for each solution method are given in the following sections.

Direct: Triangular Decomposition

The symmetric-Doolittle method of triangular decomposition solves matrix equation (254) in Cooley (1992) in a direct manner, without iteration. Details of the solution method are given in the section "Symmetric-Doolittle Method," in Cooley (1992). Briefly, the coefficient matrix A in equation (254) in

Cooley (1992) is factored into upper- and lower-triangular matrices that facilitate solution by a forward-elimination and back-substitution process. The method becomes less efficient computationally than the iterative MICCG method as the number of equations approaches the range of about 120 to 200.

Inputs for the direct-solution method consist of values for the reduced-matrix bandwidth and the condensed-matrix bandwidth. Descriptions of both bandwidths and methods for bandwidth minimization are given in the sections "Node Numbering and Determining Bandwidth" and "Techniques to Enhance Computational Efficiency." Values for the reduced-matrix bandwidth and the condensed-matrix bandwidth are input to MODFE as the program variables MBW and MBWC, respectively. Descriptions of data inputs to MODFE are given in the section "Input Instructions."

Iterative: Modified Incomplete-Cholesky Conjugate Gradient

The iterative method used to solve matrix equation (254) in Cooley (1992) is the modified incomplete-Cholesky conjugate-gradient (MICCG) method. Details of the MICCG method are given in the section "Modified Incomplete-Cholesky Conjugate-Gradient Method" in Cooley (1992), and references are given in that section for additional information about the method. In general, the coefficient matrix A of equation (254) in Cooley (1992) is split, approximately, into two matrices M and N. The factorization of M and the iterative scheme used in the MICCG method are essential to the computational efficiency of the method.

Guidelines for selecting the MICCG method over the direct method are based on the relative amounts of computer storage and execution time required for each method to solve a given aquifer problem. As stated in the previous section, the MICCG method is faster than the direct method for solving aquifer problems containing more than about 120 to 200 nodes. My experience with both methods on regular triangular meshes ranging in size from about 120 to 15,000 nodes (or equations) is that the MICCG method is about 35 to 70 percent faster than the direct method, with the larger meshes producing the greater savings in execution time.

The MICCG method uses less computer storage than the direct method when applied to meshes containing more than about 120 nodes. For meshes having fewer than about 120 nodes, the direct-solution method may use less computer storage (and time). However, the larger the aquifer problem, in number of nodes, the more favorable is the selection of the MICCG method for solution. For example, the MICCG method required about 40 percent less computer storage than the direct method for a mesh containing about 1,100 nodes. As described in previous sections, the computational efficiency of either method is related to mesh design and to the bandwidth determinations; however, the direct method is affected more by these factors than the iterative method.

The iterative MICCG method may have computational advantages over the direct method for solving nonlinear steady-state problems. As described in the section "Stopping Criteria" in Cooley (1992), the number of MICCG iterations (on an 'inner' iteration loop) can be decreased by the appropriate selection of a closure tolerance. Thus, the reduced computation time caused by taking only a few (inner) MICCG iterations may be less than the time needed to obtain a solution by the direct method. The numerical accuracy of the nonlinear solution is controlled by another closure tolerance that is placed on the outer (water-table) iterations, which are independent of, but contain, the solvers. Details about selecting a closure tolerance for the water-table iterations are given in the section "Nonlinear Conditions."

Inputs for the MICCG method consist of values for the maximum number of iterations and the closure tolerance. The maximum number of iterations is represented in MODFE as the program variable NIT, and the closure tolerance is represented as the variable TOL. Because the reduced-matrix bandwidth, MBW, is not used for the MICCG method, the maximum number of iterations, NIT, replaces MBW in the data inputs. (See section "Input Instructions.") Values for NIT are problem dependent, and usually range from about 10 to 20, for linear problems, to about 100 for nonlinear problems. The number of iterations needed for solution also is dependent on the value of the closure tolerance, TOL.

Values for the closure tolerance, TOL, are selected small enough to ensure an acceptable solution of hydraulic heads and flow rates, yet large enough to avoid excessive iteration. Usually, values for TOL range from about 0.001 to 0.0000001. The larger value is about an order of magnitude smaller than the error associated with water-level measurements, and the smaller value is near the limit of numerical accuracy for single-precision computations by most computers. For nonlinear steady-state problems, TOL should be set large enough so that closure is obtained within a few MICCG iterations. As described above, the accuracy of a nonlinear solution is controlled by an additional closure criterion for water-table iterations. Details about the operation of water-table iterations and selection of this closure criterion are given in the section "Nonlinear Conditions" and in the section "Nonlinear Case" in Cooley (1992).

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