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Chapter A5

A MODULAR FINITE-ELEMENT MODEL (MODFE) FOR AREAL AND AXISYMMETRIC GROUND-WATER-FLOW PROBLEMS, PART 3: DESIGN PHILOSOPHY AND PROGRAMMING DETAILS

By Lynn J. Torak

Book 6
MODELING TECHNIQUES

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PREFACE

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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.

CONTENTS

FIGURES

TABLES

A MODULAR FINITE-ELEMENT MODEL (MODFE) FOR AREAL AND AXISYMMETRIC GROUND-WATER-FLOW PROBLEMS PART 3: DESIGN PHILOSOPHY AND PROGRAMMING DETAILS

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. The modular structure of MODFE places the computationally independent tasks that are performed routinely by digital-computer programs simulating ground-water flow into separate subroutines, which are executed from the main program by control statements. Each subroutine consists of complete sets of computations, or modules, which are identified by comment statements, and can be modified by the user without affecting unrelated computations elsewhere in the program. Simulation capabilities can be added or modified by either adding or modifying subroutines that perform specific computational tasks, and the modular-program structure allows the user to create versions of MODFE that contain only the simulation capabilities that pertain to the ground-water problem of interest. MODFE is written in a Fortran programming language that makes it virtually device independent and compatible with desk-top personal computers and large mainframes.

MODFE uses computer storage and execution time efficiently by taking advantage of symmetry and sparseness within the coefficient matrices of the finite-element equations. Parts of the matrix coefficients are computed and stored as single-subscripted variables, which are assembled into a complete coefficient just prior to solution. Computer storage is reused during simulation to decrease storage requirements. Descriptions of subroutines that execute the computational steps of the modular-program structure are given in tables that cross reference the subroutines with particular versions of MODFE. Programming details of linear and nonlinear hydrologic terms are provided. Structure diagrams for the main programs show the order in which subroutines are executed for each version and illustrate some of the linear and nonlinear versions of MODFE that are possible. Computational aspects of changing stresses and boundary conditions with time and of mass-balance and error terms are given for each hydrologic feature. Program variables are listed and defined according to their occurrence in the main programs and in subroutines. Listings of the main programs and subroutines are given.

Introduction

This report describes the philosophy of the modular approach that was taken in designing a MODular, Finite-Element, digital-computer program (MODFE) for simulating ground-water flow in two dimensions, and the details concerning computational aspects of its simulation capabilities. It is intended to be a companion report to Part 1 (Torak, 1993), which is a user's manual that describes the simulation of ground-water flow by using MODFE, and to Part 3 (Cooley, 1992), which develops the finite-element equations that are approximated by MODFE. Simulation capabilities of MODFE are:

- 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-flux (Neumann), and head-dependent (Cauchy-type) boundary conditions,
- vertical cross sections,
- flow in axisymmetric, cylindrical coordinates (radial 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.

Background

Descriptions of the numerical representation of physical processes and hydrologic features contained

in this and the companion reports have evolved within 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.

To demonstrate the modular approach used by MODFE, the computational steps that are required to simulate any ground-water flow problem are arranged into an ordered list or a generalized flow chart. Subroutines are listed in tables according to the computational steps that are performed, and brief descriptions of the subroutines are given. Versions of MODFE that require each subroutine also are indicated in the tables for reference.

Hydrologic terms are grouped into two categories: linear and nonlinear, and programming details for each group are given. These details, together with the variable lists and definitions, allow the interested user to modify the existing simulation capabilities of MODFE or to create additional capabilities.

Computational aspects of steady-state flow, changing stresses and boundary conditions with time, and of the water-balance summary are described to give the user necessary background information for either invoking these simulation capabilities or identifying the location within the program where computations occur. Details of computations within the equation-solving subroutines are provided to demonstrate how the theoretical development described in Cooley (1992) is put into practice with MODFE.

Methods of computer-storage allocation and usage that enhance the efficiency of MODFE are explained by using tables and diagrams. These descriptions are provided to promote an understanding of details of program design and to allow the user to add or modify simulation capabilities that are consistent with the design philosophy.

Purpose and Scope

This report provides technical details about the modular-program structure and about specific computations for simulation capabilities of MODFE. Discussions of modules, either sets of subroutines that add a particular simulation capability to MODFE, or sets of complete mathematical computations within subroutines, are kept brief, but are presented to familiarize the user with the overall philosophy of program design. Descriptions of how and where specific computational tasks are performed within MODFE, and definitions of corresponding program variables, are provided so that a user can follow the progression of computations that are required to transform the mathematical expressions described in Cooley (1992) into a working computer program. Together with lists of the main programs and subroutines, these descriptions and definitions provide the user with background information that is necessary for modifying existing simulation capabilities, adding new capabilities, or simply using MODFE in an appropriate manner to solve a particular ground-water-flow problem.

Design Philosophy for a Modular Approach

The philosophy behind designing MODFE was to construct a digital-computer model of two-dimensional ground-water flow in which the independent computational steps that are necessary for simulation are contained in separate subroutines (fig. 1). The delineation of computational steps by subroutines is termed a modular approach. The order in which these steps are executed is controlled by a main program. Simulation capabilities and matrix-equation solvers are modified or added to the model by either modifying or adding subroutines and their controlling statements to the program. Consequently, a user can construct different versions of MODFE that contain different simulation capabilities and solvers, depending on the subroutines that are included (or excluded) in the program structure, and on the arrangement of controlling statements to subroutines in the main programs. Program structures for versions of MODFE that are possible with the modular approach are described in a later section.

Modules and Subroutines

The modular approach and design philosophy described above for the main programs were applied to the subroutines. Each subroutine consists of one or several sets of program statements (or modules) that perform a specific task. Each module requires specific input from the previous module, and all modules function to complete one of the computational steps shown in figure 1. For example, two modules within the subroutine that forms coefficients to matrix equations (subroutine FMCO) are: 1) computing the coefficients for coordinate functions and, 2) computing the element contribution to distributed recharge or discharge. The coordinate functions from the first module are used to compute element areas, which are used in the second module to compute the coefficient for distributed recharge or discharge. Modules are defined in the subroutines by comment statements

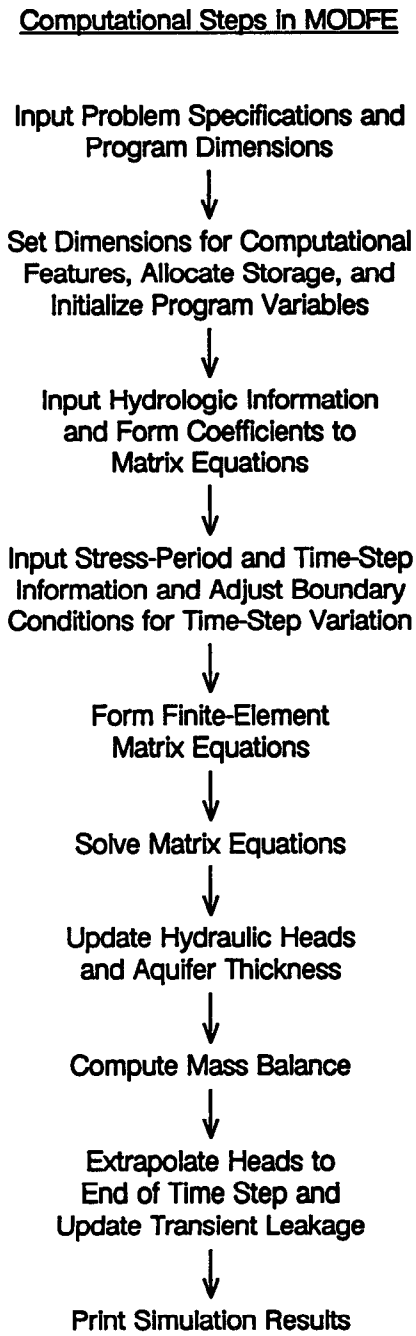

Figure 1.—Diagram of generalized flow chart showing computational steps performed by subroutines of MODular Finite-Element model (MODFE).

and may be modified by the user to suit the specific needs of an aquifer problem. A listing of subroutines is given in the Appendices.

Efficient Use of Computer Storage and Processing Time

Another design consideration in the development of MODFE was the efficient use of computer storage and processing time. MODFE was designed to be compatible with computers that have small core storage, such as minicomputers or personal computers (PC's). All information is stored and processed either as single-subscripted variables (vector storage) or as unsubscripted variables; there are no multidimensional variables (array storage) used in MODFE. A general-storage vector, G, is used to store the vector lengths, and computer storage for each vector length is determined at the time of execution of MODFE. Storage locations within G are reused routinely during simulation to decrease storage requirements. Details about storage locations in G are given in the section "General-Storage Vector G."

Coefficients to matrix equations are formed and stored in a manner that uses computer storage and processing time efficiently. The information needed to assemble matrix equations for a node is stored as close together in the computer as physically possible. This storage scheme decreases the amount of transferring of information into and out of computer memory (commonly known as paging). Further decreases in computer storage and processing time are realized by eliminating equations at specified-head nodes from the matrix equation that is solved. Details of these processes are given in subsections of the section "Allocation of Computer Storage and Processing Time."

Device-Independent Programming

MODFE has been programmed in USA Standard Fortran, defined by the American National Standards Institute, Incorporated (ANSI) as standard USAS ×3.9–1966, commonly termed Fortran 66. No extensions to this programming language that may be available from a particular computer manufacturer have been used in MODFE. However, each computer installation may require unique statements for program identification or for allocating large amounts of vector storage. For example, to use MODFE on the PRIME computer, the general-storage vector G has been placed in a Fortran COMMON statement.

Adherence to the ANSI standard Fortran 66 allows MODFE to be used on many different types of computers. During development, MODFE had been used on at least eight different computers, including minicomputers and PC's. Each computer contained either different storage lengths for single-precision variables or either virtual or nonvirtual memory. Simulations on these computers produced nearly identical results,

Table 1.—Linear versions of MODular Finite-Element model (MODFE) and simulation capabilities

Simulation capabilities of linear versions of MODFE	
Nonhomogeneous, anisotropic flow having changing directions of anisotropy within the model region Steady vertical leakage (no storage effects) Point and areally distributed sources and sinks Specified head (Dirichlet), specified flux (Neumann), and head-dependent (Cauchy-type) boundary conditions	Axisymmetric (radial) flow Zoned input of hydraulic properties and boundary conditions Nonsteady-state or steady-state conditions Vertical cross sections Changing stresses and boundary conditions with time

Simulation options	Solver options	
	Direct, symmetric-Doolitle method	Iterative, MICCG method
Steady vertical leakage (no storage effects)	LMFE1	LMFE2
Vertical leakage having storage effects (transient leakage)	LMFE3	LMFE4

and only slight modifications were required at the beginning of the programs, as described above. Thus, MODFE is programmed to be as device independent as possible.

Simulation Capabilities and Versions of MODular Finite-Element Model (MODFE)

The versions of MODFE that are possible from the modular program design are divided among three classes of ground-water-flow problems: (1) linear, steady or nonsteady state, (2) nonlinear, nonsteady state, and (3) nonlinear steady state. The linear versions of MODFE simulate hydrologic processes in which the equation formulation is unchanged during simulation. A list of linear versions and simulation capabilities is given in table 1. The nonlinear versions of MODFE simulate hydrologic processes with complex equation formulations that change during simulation. Separate nonlinear versions were constructed for steady- and nonsteady-state conditions because of the unique equation formulation required to simulate these types of ground-water-flow problems. Simulation capabilities of the nonlinear versions are listed in table 2 for nonsteady-state conditions and in table 3 for steady-state conditions.

Each version of MODFE contains different options for simulation capabilities and for solution methods to the finite-element matrix equations. Hence, simulation or solution options create different structures of the main program and different versions of MODFE. Selection of options and program structures is user dependent; that is, the user determines which simulation or solution options are applicable to the ground-water-flow problem and constructs an appropriate version of MODFE. Structures of main programs to the versions listed in tables 1–3 are given in the following section. Details of using the simulation capabilities are given in Torak (1993).

Table 2.—Nonlinear versions of MODular Finite-Element model (MODFE) and simulation capabilities

Simulation capabilities of nonlinear versions of MODFE	
Nonhomogeneous, anisotropic flow having changing directions of anisotropy within the model region Steady vertical leakage (no storage effects) Point and areally distributed sources and sinks Specified head (Dirichlet), specified flux (Neumann), and head-dependent (Cauchy-type) boundary conditions Axisymmetric (radial) flow	Zoned input of hydraulic properties and boundary conditions Nonsteady-state conditions Unconfined (water-table) conditions Partial drying and resaturation of a water-table aquifer Conversion between confined- and unconfined-aquifer conditions Change stresses and boundary conditions with time

Simulation options	Solver options	
	Direct, triangular-decomposition method	Iterative, MICCG method
Steady vertical leakage (no storage effects)	NLMFE1	NLMFE2
Vertical leakage having storage effects (transient leakage)	NLMFE3	NLMFE4
Nonlinear steady vertical leakage	NLMFE5	NLMFE6
Nonlinear head-dependent (Cauchy-type) boundaries	NLMFE7	NLMFE8

The following naming convention is adopted to identify each version of MODFE. The four linear versions listed in table 1 are termed LMFEn for "Linear Modular Finite Element, version n," where n = 1–4. The eight nonlinear versions listed in table 2 are termed NLMFEn for "NonLinear, Modular Finite Element, version n," where n = 1–8. The six nonlinear steady-state versions listed in table 3 are termed NSSFEn for "Nonlinear, Steady-State, Finite-Element, version n," where n = 1–6. Note that the linear versions of MODFE simulate nonsteady-state and steady-state conditions, whereas separate versions are used for the nonlinear conditions.

Program Structures and Lists of Main Programs

The order in which subroutines are executed and computational steps are performed by the main programs is shown diagrammatically in figures 2–12 for the versions of MODFE listed in tables 1–3. Each subroutine name shown in the structure diagrams represents one or more computational steps in the generalized flow chart of figure 1. The computational steps corresponding to each subroutine are described in tables in the following section, and the versions of MODFE that use each subroutine are indicated in the tables for reference. Subroutine names in the structure diagrams are replaced by Fortran CALL statements to form the main programs. Computer listings of main programs and subroutines are given in the Appendices.

Subroutine names that are linked to the main programs by dashed lines in the structure diagrams contain the simulation options listed in tables 1–3. The Fortran CALL statements to these subroutines are inserted into the main program according to the order indicated by the structure diagrams, and the corresponding subroutines are added to MODFE for compilation. Thus, if a simulation capability defined by these subroutines is not required for the aquifer problem, then the Fortran CALL statements and the corresponding subroutines are removed from the program creating a version of MODFE having a new program structure.

Table 3.—Nonlinear steady-state versions of MODular Finite-Element model (MODFE) and simulation capabilities

Simulation capabilities of nonlinear versions of MODFE	
Nonhomogeneous, anisotropic flow with changing directions of anisotropy within the model region Steady vertical leakage (no storage effects) Point and areally distributed sources and sinks Specified head (Dirichlet), Specified flux (Neumann), and head-dependent (Cauchy-type) boundary conditions Axisymmetric (radial) flow	Zoned input of hydraulic properties and boundary conditions Steady-state conditions Unconfined (water-table) conditions Partial drying and resaturation of a water-table aquifer Conversion between confined- and unconfined-aquifer conditions

Simulation options	Solver options	
	Iterative, MICCG method	Direct, triangular-decomposition method
Water-table conditions only	NSSFE1	NSSFE2
Nonlinear steady vertical leakage	NSSFE3	NSSFE4
Nonlinear head-dependent (Cauchy-type) boundaries	NSSFE5	NSSFE6

Subroutine names appearing in parentheses in the structure diagrams replace those that are located beside them in the structure. For example, in figure 2, subroutines required for the iterative, MICCG, solution method (subroutines INITCG, SETCG, and MICCG) replace subroutines used for the direct method (subroutines INITB, SETB, and BAND). This replacement creates another version of MODFE, which is indicated by the program name in parentheses at the top of the structure diagram (LMFE2 in this example).

Two additional program structures result from combining simulation capabilities of the nonlinear versions (figs. 8 and 12). The program structure shown in figure 8 represents a nonsteady-state version of MODFE that can simulate nonlinear steady vertical leakage, nonlinear head-dependent (Cauchy-type) boundaries, and nonlinear point sinks. A steady-state version of MODFE having the same simulation capabilities as the version shown in figure 8 is represented by the structure diagram in figure 12. Note that the order in which Fortran CALL statements are added to the main program determines the order of inputs and other computations for these features. Therefore, although subroutines for nonlinear steady vertical leakage (subroutine names that begin with "VN") can be called by the main program before subroutines for nonlinear head-dependent (Cauchy-type) boundaries and nonlinear point sinks (subroutine names that begin with "GN"), this new order of subroutines in the main program is not consistent with the order of inputs given in the input instructions in Torak (1993). To preserve the order of inputs as given in Torak (1993), the main programs for these versions of MODFE should be structured according to the diagrams in figures 8 and 12.

Computational Steps and Subroutines

The computational steps shown in the generalized flow chart (fig. 1) are performed in each version of MODFE by subroutines that are accessed from the main programs (listed in the previous section). The purpose of each subroutine can be identified from their names. Subroutine names contain groups of letters that function as identifiers for either the simulation capability or the computational step that is performed. A list of identifiers and the corresponding computational step or simulation capability is given in table 4.

Descriptions of the computational steps performed by each subroutine in MODFE are given in tables 5–14. Subroutines are listed according to the compu-

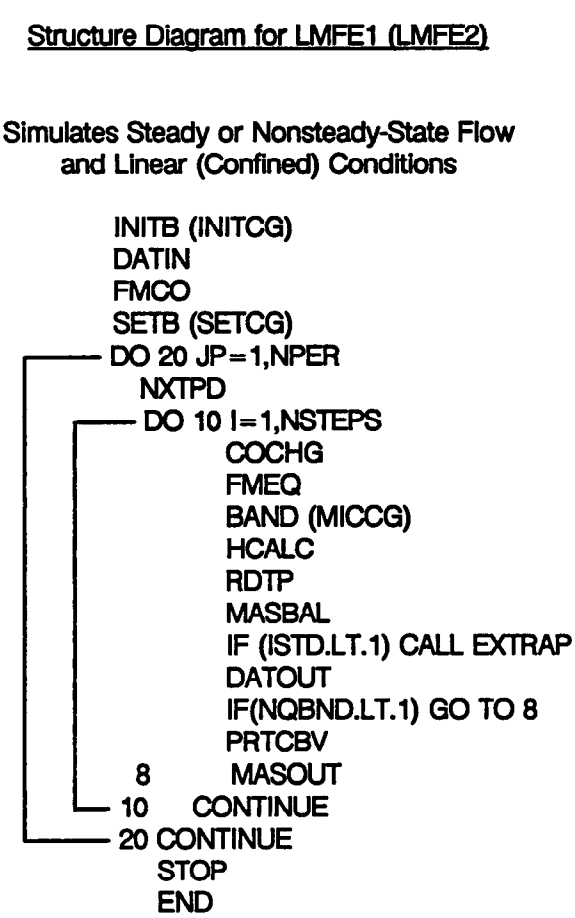

Figure 2.—Main-program structure for MODular Finite-Element model (MODFE) version LMFE1 (LMFE2), simulates steady or nonsteady-state flow and linear (confined) conditions.

tational steps in the generalized flow chart (fig. 1). Versions of MODFE that require a subroutine are indicated by x's in the tables. Subroutines that are required by the versions listed in parentheses are indicated by the symbol (x). Subroutines that perform utility-type functions, such as printing or reading information and computing the reduced-matrix bandwidth (see section "Reduced Matrix A"), are given in table 15.

Programming Details of Linear Hydrologic Terms

The following sections give programming details about mathematical processes and computations that pertain to input and to the formation of coefficients and equations for the linear versions of MODFE (table 1). Additional details concerning specific computations or inputs are given with the program-variable descriptions in the appendices and in sections of Torak (1993) that describe the corresponding simulation capability. A development of the equations referenced in the following sections is contained in Cooley (1992).

Descriptions of the programming details for linear hydrologic terms in MODFE refer to the finite-element matrix equations for steady- and nonsteady-state conditions frequently; thus, these equations are restated here for reference. For nonsteady-state conditions, the finite-element matrix equation is given by equation (58) in Cooley (1992):

$$\left(\frac{\underline{\underline{C}}}{\left(\frac{2}{3}\right)\Delta t_{n+1}}\right)\underline{\delta}=\underline{B}-\underline{\underline{A}}\hat{h}_n \qquad (1)$$

For steady-state conditions, the finite-element matrix equation is given by equation (232) in Cooley (1992):

$$\underline{\underline{A}}\,\underline{\delta}_0=\underline{B}-\underline{\underline{A}}\,\underline{h}_0 \qquad (2)$$

Terms contained in equations (1) and (2) are defined by the following equations in Cooley (1992): the C and A matrices and the B vector are defined by equations (46)–(50), for Cartesian coordinates, and by equations (224)–(229) for axisymmetric cylindrical coordinates, δ is defined by equation (57), and δ_0 and h_0 are defined in equation (231) and subsequent discussion. Programming details of the linear components of the C and A matrices and of the B vector are described in the following sections.

Transmissivity

Transmissivity terms are computed in subroutine FMCO according to equation (43) in Cooley (1992). These terms represent element contributions to the off-diagonal transmissivity coefficients in the G matrix, which, together with the V matrix, comprise the matrix A in equations (1) and (2) (see development in Cooley (1992) leading to equation (46)). Values for the local x and y transmissivity tensor, $T_{\bar{x}\bar{x}}$ and $T_{\bar{y}\bar{y}}$, are input by hydraulic-property zone as program variables XTR and YTR, respectively. The transmissivity values are first multiplied (scaled) by 0.5, then divided by twice the element area, represented as program variable AREA, before being multiplied by the coordinate functions $\bar{b}_i$, $\bar{b}_j$, $\bar{c}_i$, and $\bar{c}_j$ to create the transmissivity terms. The coordinate functions and the transmissivity terms are computed by using coordinates that have been rotated from the global x–y system to the local $\bar{x}$–$\bar{y}$ system. Transmissivity terms

Structure Diagram for LMFE3 (LMFE4)

Simulates Steady or Nonsteady-State Flow, Linear (Confined) Conditions and Vertical Leakage of Water Stored Elastically in a Confining Bed (Transient Leakage)

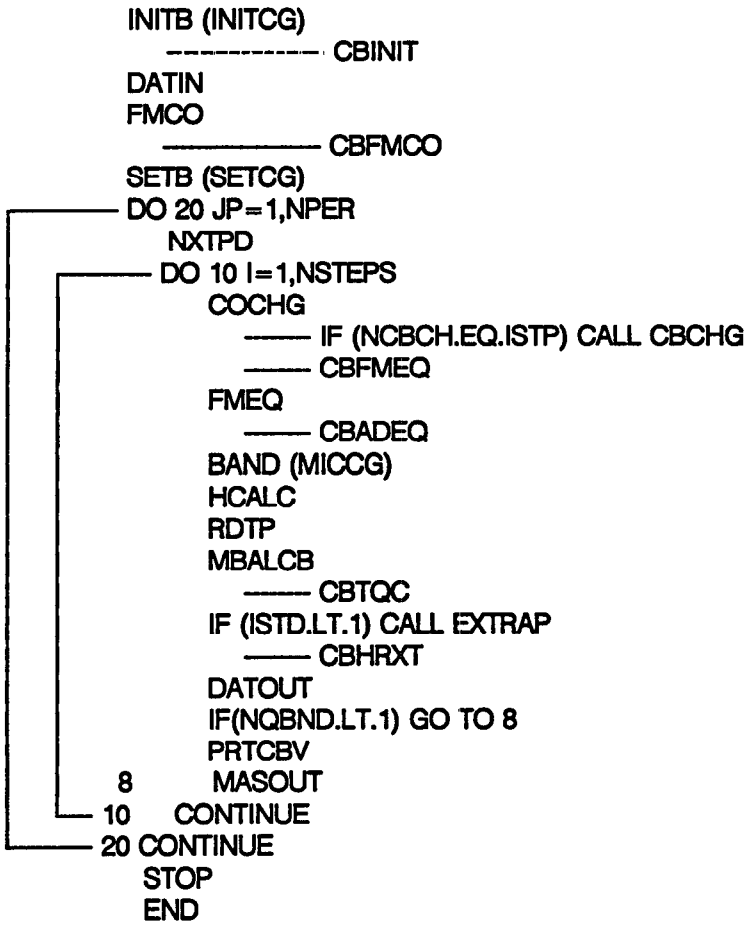

Figure 3.—Main-program structure for MODular Finite-Element model (MODFE) version LMFE3 (LMFE4), simulates steady or nonsteady-state flow, linear (confined) conditions and vertical leakage of water stored elastically in a confining bed (transient leakage).

are computed for each node in the element, and are represented by the program variables TFL(i), where i = 1–3.

For axisymmetric (radial) flow, the computations described above are performed by using values of hydraulic-conductivity in the radial (XTR) and vertical (YTR) directions. The hydraulic conductivity terms are multiplied by the centroidal radius of the element in subroutine FMCO to obtain the element contribution to the transmissivity coefficient for each node. The centroidal radius is computed as the arithmetic mean of the r coordinates, which are input and stored in MODFE as the vector XG. The element contributions (TFL terms) are summed according to equation (49) in Cooley (1992) to yield the coefficients, which are stored in the appropriate locations for each node in the program vector A. Because of symmetry in the G matrix and properties of the coordinate functions, the summations involve only transmissivity terms that link a node in the matrix equation to higher-numbered nodes. Details about the coordinate functions and the symmetry of the G matrix are given in Cooley (1992). Because the transmissivity coefficients to the G matrix are stored in the vector A, the element contributions (TFL terms) for each node are not stored within MODFE.

Structure Diagram for NLMFE1 (NLMFE2)

Simulates Nonsteady-State Flow and Unconfined (Water-Table) Conditions

```
INITB (INITCG)
WTINIT
DATIN
FMCO
WTFMCO
SETB (SETCG)
DO 20 JP=1,NPER
   NXTPD
   DO 10 I=1,NSTEPS
      COCHG
      RDTP
      FMEPWT
      BAND (MICCG)
      HCALWT
      RDTP
      FMECWT
      BAND (MICCG)
      WTCCHK
      IF (ISC.EQ.0) GO TO 5
      HCALWT
      RDTP
      FMECWT
      BAND (MICCG)
5     HCALWT
      RDTP
      MBALWT
      IF (ISTD.LT.1) CALL XTRPWT
      DATOUT
      IF(NQBND.LT.1) GO TO 8
      PRTCBV
8     MASOUT
10  CONTINUE
20 CONTINUE
   STOP
   END
```

Figure 4.—Main-program structure for MODular Finite-Element model (MODFE) version NLMFE1 (NLMFE2), simulates nonsteady-state flow, and unconfined (water-table) conditions.

Structure Diagram for NLMFE3 (NLMFE4)

Simulates Nonsteady-State Flow, Unconfined (Water-Table) Conditions, and Vertical Leakage of Water Stored Elastically in a Confining Bed (Transient Leakage)

```
INITB (INITCG)
WTINIT
   ---------- CBINIT
DATIN
FMCO
WTFMCO
                ---------- CBFMCO
SETB (SETCG)
NXTPD
DO 20 JP=1,NPER
   NXTPD
   DO 10 I=1,NSTEPS
      COCHG
         ------- IF (NCBCH.EQ.ISTP) CALL CBCHG
      RDTP
         ------ CBFMEQ
      FMEPWT
         ------ CBADEQ
      BAND (MICCG)
      HCALWT
      RDTP
      FMECWT
         ------ CBADWT
      BAND (MICCG)
      WTCCHK
      IF (ISC.EQ.0) GO TO 5
      HCALWT
      RDTP
      FMECWT
         ------ CBADWT
      BAND (MICCG)
5     HCALWT
      RDTP
      MBWTCB
         ------ CBTQC
      IF (ISTD.LT.1) CALL XTRPWT
         ------- CBHRXT
      DATOUT
      IF(NQBND.LT.1) GO TO 8
      PRTCBV
8     MASOUT
10  CONTINUE
20 CONTINUE
   STOP
   END
```

Figure 5.—Main-program structure for MODular Finite-Element model (MODFE) version NLMFE3 (NLMFE4), simulates nonsteady-state flow, unconfined (water-table) conditions, and vertical leakage of water stored elastically in a confining bed (transient leakage).

The transmissivity coefficients are used to form parts of the G matrix in finite-element equations (1) and (2) in subroutine FMEQ. The off-diagonal terms that were stored in the program vector A by node in subroutine FMCO are written to other storage locations within the A vector that represent off-diagonal entries of the G matrix. The off-diagonal entries are identified by the storage locations A(NME+J). The transmissivity coefficient for the main diagonal is assembled by summing the negative values of the off-diagonal terms according to equation (43) in Cooley (1992) and storing the sum in the program vector AD for each node. After the matrix components are assembled for all equations, the main-diagonal terms are written to the storage locations A(NME) in the A vector.

Structure Diagram for NLMFE5 (NLMFE6)

Simulates Nonsteady-State Flow, Unconfined (Water-Table) Conditions, and Nonlinear Steady Vertical Leakage

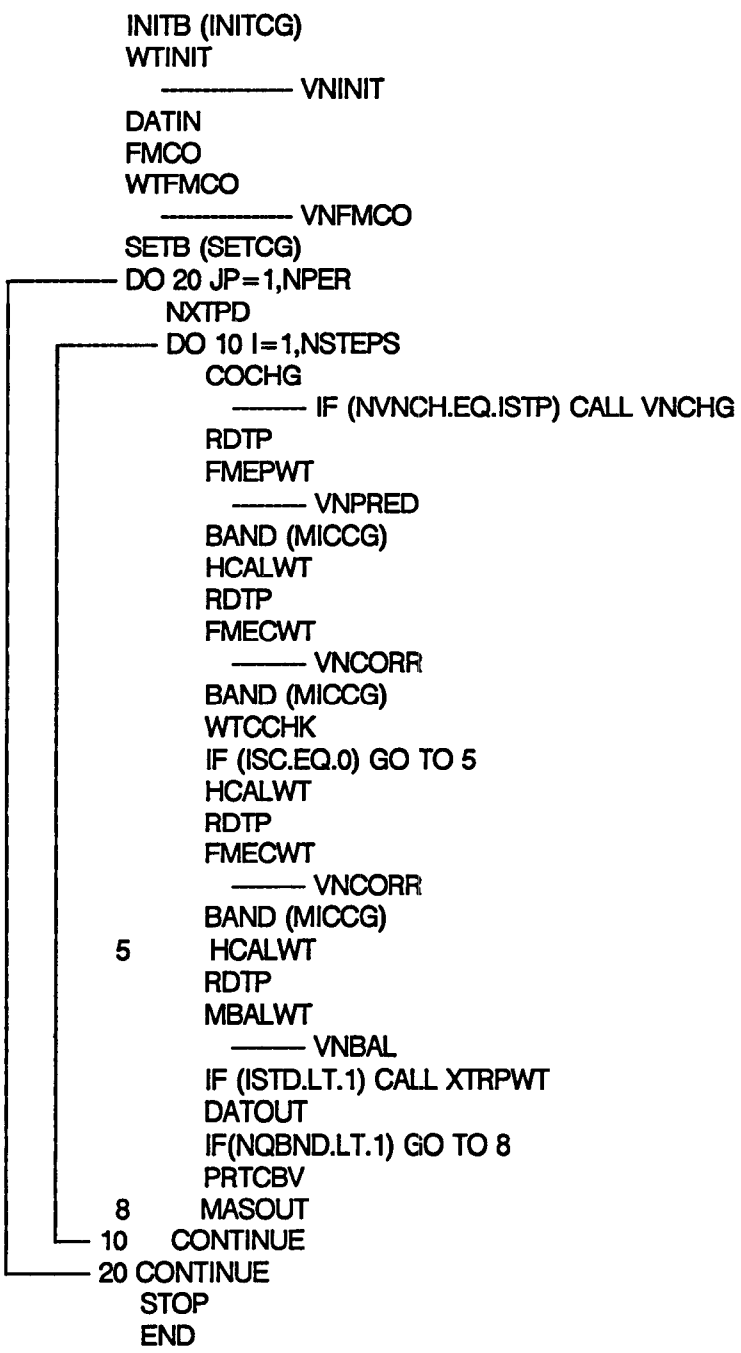

Figure 6.—Main-program structure for MODular Finite-Element model (MODFE) version NLMFE5 (NLMFE6), simulates nonsteady-state flow, unconfined (water-table) conditions, and nonlinear steady vertical leakage.

Structure Diagram for NLMFE7 (NLMFE8)

Simulates Nonsteady-State Flow, Unconfined (Water-Table) Conditions, Nonlinear Head-Dependent (Cauchy-type) Boundaries, and(or) Nonlinear Point Sinks

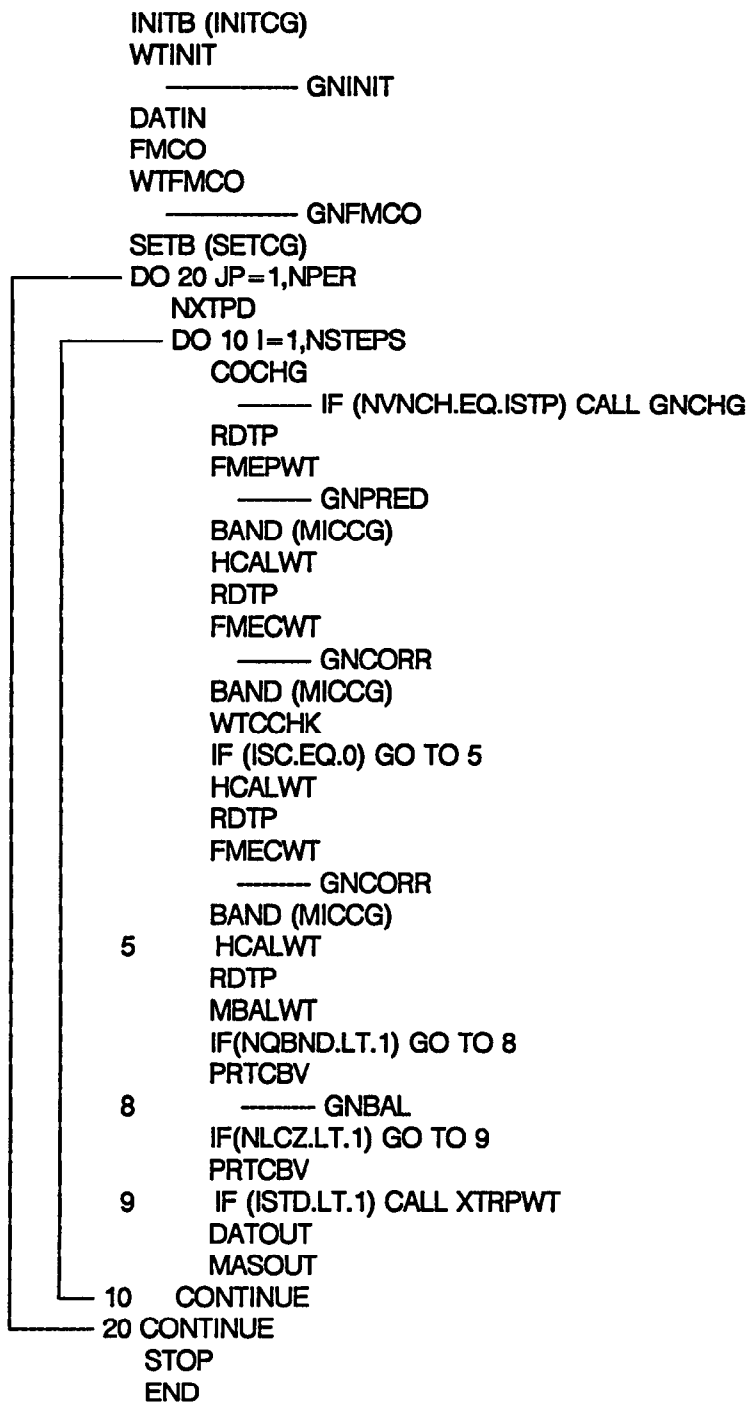

Figure 7.—Main-program structure for MODular Finite-Element model (MODFE) version NLMFE7 (NLMFE8), simulates nonsteady-state flow, unconfined (water-table) conditions, nonlinear head-dependent (Cauchy-type) boundaries, and (or) nonlinear point sinks.

Structure Diagram for NLMFE5 (NLMFE6) Combined with NLMFE 7 (NLMFE8)

Simulates Nonsteady-State Flow, Unconfined (Water-Table) Conditions, Nonlinear Head-Dependent (Cauchy-type) Boundaries and (or) Nonlinear Point Sinks, and Nonlinear Steady Vertical Leakage

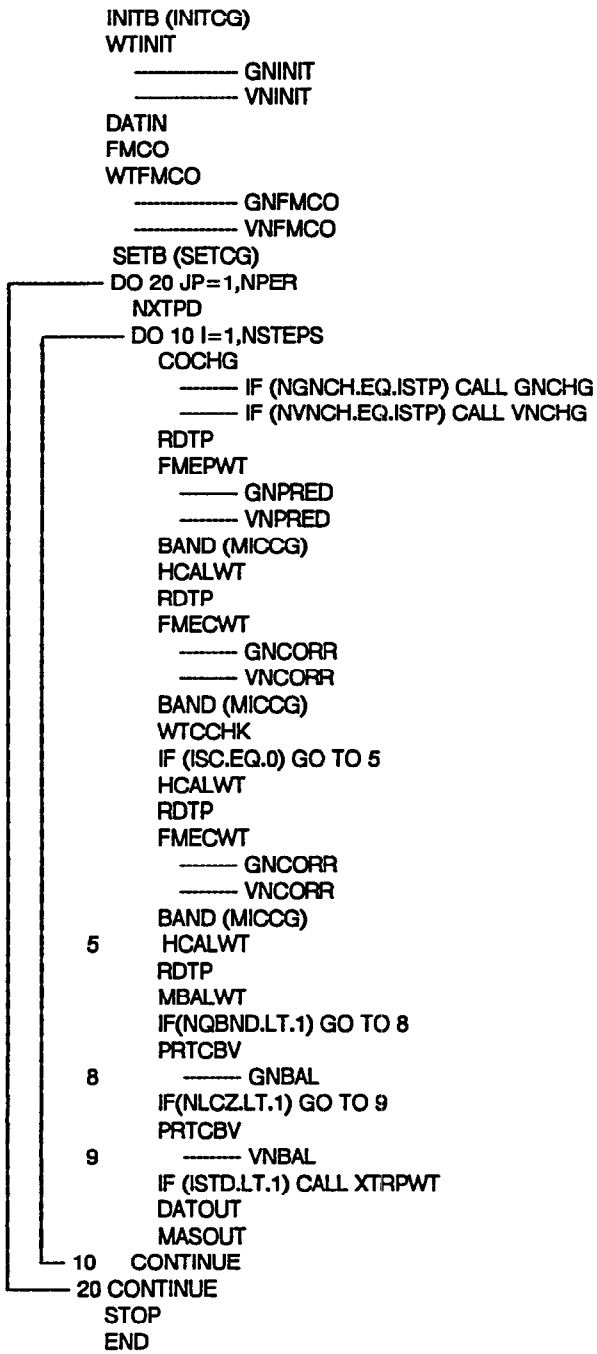

Figure 8.—Main-program structure for MODular Finite-Element model (MODFE) version NLMFE5 (NLMFE6) combined with NLMFE7 (NLMFE8), simulates nonsteady-state flow, unconfined (water-table) conditions, nonlinear head-dependent (Cauchy-type) boundaries and (or) nonlinear point sinks, and nonlinear steady vertical leakage.

Structure Diagram for NSSFE1 (NSSFE2)

Simulates Steady-State Flow and Unconfined (Water-Table) Conditions

```
INITCG (INITB)
SWINIT
DATIN
FMCO
SETCG (SETB)
SWFMCO
DO 50 IT=1,NITSW
    FMEQ
    MICCG (BAND)
    SWBDMP
    HCALC
    RDTP
    SWTHK
    IF (DSPA.LT.TOLSW) GO TO 60
50 CONTINUE
60 MASBAL
   DATOUT
   TKOUT
   IF(NQBND.LT.1) GO TO 62
   PRTCBV
62 MASOUT
   STOP
   END
```

Figure 9.—Main-program structure for MODular Finite-Element model (MODFE) version NSSFE1 (NSSFE2), simulates steady-state flow and unconfined (water-table) conditions.

Structure Diagram for NSSFE3 (NSSFE4)

Simulates Steady-State Flow, Unconfined (Water-Table) Conditions, and Nonlinear Steady Vertical Leakage

```
INITCG (INITB)
SWINIT
   ---------- VNINIT
DATIN
FMCO
SETCG (SETB)
SWFMCO
   ---------- VNFMCO
DO 50 IT=1,NITSW
    FMEQ
    ---------- VNPRED
    MICCG (BAND)
    SWBDMP
    HCALC
    RDTP
    SWTHK
    IF (DSPA.LT.TOLSW) GO TO 60
50 CONTINUE
60 MASBAL
   ---------- VNBLSS
   DATOUT
   TKOUT
   IF(NQBND.LT.1) GO TO 62
   PRTCBV
62 MASOUT
   STOP
   END
```

Figure 10.—Main-program structure for MODular Finite-Element model (MODFE) version NSSFE3 (NSSFE4), simulates steady-state flow, unconfined (water-table) conditions, and nonlinear steady vertical leakage.

Note that program vector A is used in subroutine FMEQ to assemble all components of the C and G matrices in the finite-element matrix equations and in subroutines BAND or MICCG for solution of the matrix equations. The manner in which storage locations in the A vector are allocated and reused during completion of other computational steps is described in the section "Allocation of Computer Storage and Processing Time."

Storage Coefficient

Inputs and computations for the storage-coefficient terms are performed in subroutine FMCO. The artesian storage coefficient is input by hydraulic-property zone as the program variable STR. The storage-coefficient terms are computed according to equation (36) in Cooley (1992). Values of STR are multiplied (scaled) by the square of the scaling factor for nodal coordinates (program variable SCALE) and divided by 6 to account for use of scaled values for nodal coordinates and to permit a subsequent multiplication of STR by twice the element area (program variable AREA). Multiplication of STR by AREA yields the storage-coefficient term, c^e_{ii} of equation (36) in Cooley (1992), for node i in element e. These terms represent contributions to the C matrix of equations (1) and (2) for each node in the element and are represented by program variables TESJ, TESK, and TESL. Values of TESJ, TESK, and TESL are identical in simulations that use Cartesian coordinates. For axisymmetric cylindrical coordinates, the element contributions to the C matrix are multiplied by the centroidal radius associated with one-third of the element area that corresponds to each node.

Element contributions to the C matrix coefficients (TESJ, TESK, and TESL terms) are summed by node

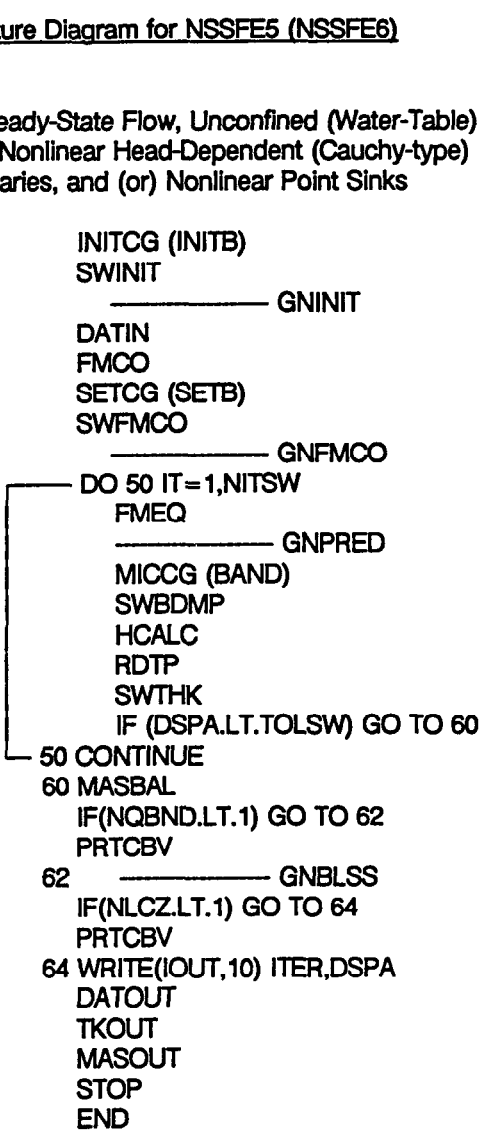

Figure 11.—Main-program structure for MODular Finite-Element model (MODFE) version NSSFE5 (NSSFE6), simulates steady-state flow, unconfined (water-table) conditions, nonlinear head-dependent (Cauchy-type) boundaries, and (or) nonlinear point sinks.

in subroutine FMCO according to equation (47) in Cooley (1992). The sums represent the main-diagonal entries to the C matrix of equation (1) and are stored for each node in the A vector. The main-diagonal entries for each node in an element are identified in program vector A by the storage locations A(ICA), A(ICB), and A(ICC).

The storage-coefficient terms are assembled into finite-element matrix equation (1) in subroutine FMEQ. The main-diagonal terms are identified during the assembly by the storage locations A(NC) in program vector A. Values in the A(NC) locations for each equation are divided by (2/3)Δt and summed into other storage locations in program vector A, A(NME), which represent the main diagonals of the C, V, and G matrices of the matrix equations.

Steady Vertical Leakage

Terms for steady vertical leakage (no storage effects from a confining bed) are computed in subroutine FMCO in the manner expressed by the R^e term of equation (37) in Cooley (1992). The vertical hydraulic conductance of the confining bed (vertical hydraulic conductivity divided by confining-bed thickness), R^e, is input to MODFE in subroutine FMCO by hydraulic property zone as the program variable VLC. This value is multiplied (scaled) by the square of the scaling factor, SCALE, for length terms, and divided by 6 to allow subsequent multiplication by AREA, which has been described previously in the section "Storage Coefficient." The multiplication by AREA creates the steady-vertical leakage term, $(1/3)R^e\Delta^e$, which is used to form part of the diagonal entry of matrix V, v^e_{kk} of equation (37) in Cooley (1992), for each node k in element e. This term is represented by program variable TEL, and is the element contribution from each node to the V matrix of equations (46) and (48) in Cooley (1992).

The element contributions, TEL, are summed by node in subroutine FMCO to create the steady leakage coefficient, V_{ij}, of equation (48) in Cooley (1992). The sum is stored in one storage location within the A vector for each node for assembly into a finite-element matrix equation by subroutine FMEQ. Details about storage of matrix components and assembly of the matrix equation are given in the section "Allocation of Computer Storage and Processing Time." With the V matrix coefficients computed and stored in the A vector, the vertical hydraulic conductances (TEL terms) from each element are not required for further processing; hence, they are not stored in MODFE.

Vertical Leakage of Water Stored Elastically in a Confining Bed

Terms used to simulate vertical leakage of water stored elastically in a confining bed, or transient leakage, are computed in subroutine CBFMCO. The steady vertical leakage component of transient leakage is not computed in this subroutine. Instead, the terms A, α, B, and β, which are used to approximate transient leakage functions $M_1(\Delta t_d)$ and $M_2(\Delta t_d)$ of equations (188) and (189), respectively, in Cooley (1992), are assigned values in subroutine CBFMCO. These terms are represented, respectively, by

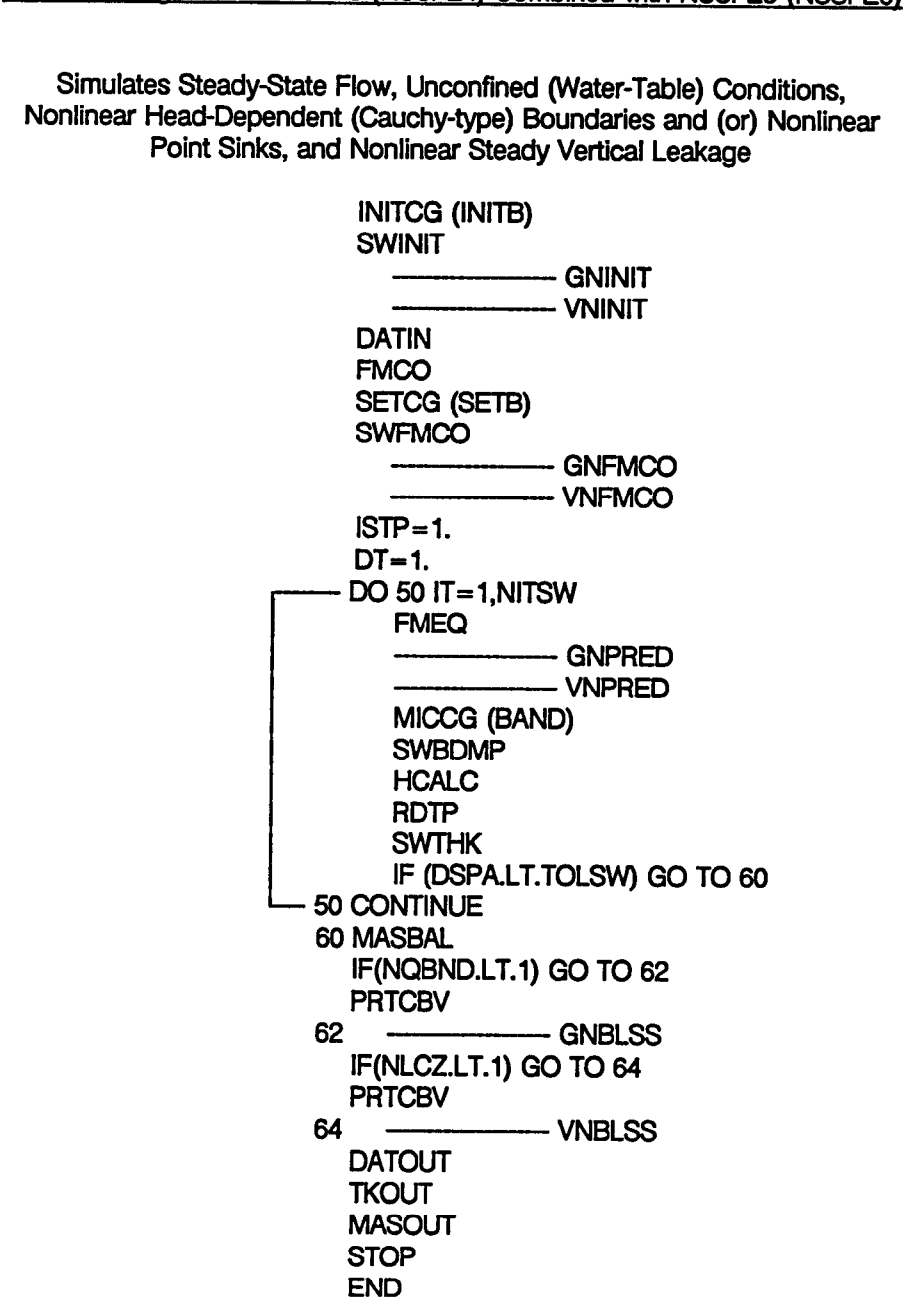

Figure 12.—Main-program structure for MODular Finite-Element model (MODFE) version NSSFE3 (NSSFE4) combined with NSSFE5 (NSSFE6), simulates steady-state flow, unconfined (water-table) conditions, nonlinear head-dependent (Cauchy-type) boundaries and (or) nonlinear point sinks, and nonlinear steady vertical leakage.

program vectors AC, ALF, BC, and BTA. Values for the effective vertical hydraulic conductivity and the effective specific storage of the confining bed, expressed by the summations in the numerator and denominator, respectively, of equation (167) in Cooley (1992) are computed as an intermediate step to computing nodal values of γ_i of this equation. The effective vertical hydraulic conductivity at a node in element e, $(1/3)K_{zz}'^{e}\Delta^{e}$, is computed as the program variable TEVC. These values are summed by element for each node and are stored in the program vector WVCN. Likewise, the effective specific storage, $(1/3)S_s'^{e}\Delta^{e}$,

Table 4.—Naming convention for subroutines

Identifier	Computational step
B	Solves matrix equations by using the direct symmetric-Doolittle method.
CG	Solves matrix equations by using the iterative conjugate-gradient method.
CHG	Adjust or change stresses and boundary conditions (table 8).
EQ, FME PRED, CORR	Form finite-element matrix equations (table 9).
FMCO	Form coefficients to matrix equations (table 7).
HCAL	Update hydraulic heads (table 11).
INIT	Input problem specifications and initialize program variables (tables 5 and 6).
MAS, BAL MB, BL	Compute mass balance (table 12).
OUT, PRT	Print hydrologic information and simulation results.
XT	Extrapolate heads to end of time step (table 13).
	Simulation capability
CB	Vertical leakage with storage effects (transient leakage).
GN	Nonlinear head-dependent (Cauchy-type) boundaries and nonlinear point sinks.
SS, SW	Nonlinear, steady-state conditions.
VN	Nonlinear steady vertical leakage.
WT	Water-table conditions.

for a node in element e is computed as the program variable TESA, summed by element for each node, and stored temporarily as the program vector GMA. These values are combined with the steady vertical leakage coefficient, $(1/3)R^e\Delta^e$, discussed in the previous section, to create the γ_i term. This computation is performed only if the value of the effective specific storage (stored in GMA) is greater than "zero," as transient leakage can occur only if the specific storage is nonzero. The zero condition for specific storage is evaluated by MODFE at 10^{-30}, where γ_i is computed if the effective specific storage is larger than this value. Values of γ_i are computed and stored in the vector GMA to be used later in forming the finite-element matrix equations.

Computations for the exponential series M_1 and M_2 are performed in subroutine CBFMEQ. The series M_1 is represented as the program variable SM1. Values of SM1 are used later in this subroutine to form the term C_h of equation (203) in Cooley (1992), which is part of the A matrix of equation (1). The series M_2 is not represented by program variables; instead, its computation is contained within computations for other transient-leakage terms, discussed below.

Parts of the transient leakage flux given by the P and Q terms of equations (199)–(202) and the term C_H given by equation (204) in Cooley (1992) are computed for each node and are represented by the program vector CBQ in subroutine CBFMEQ. Terms in P that correspond to the series M_1 are computed and stored in the program vector QOM1(NT) for each term NT of the series. Likewise, terms in P that correspond to the series M_2 are represented by the program vector QOM2(NT). These values represent the transient

Table 5.—Subroutines that input problem specifications and program dimensions

Subroutine	Description of input	Versions of MODFE that require subroutine								
		LMFE1 (LMFE2)	LMFE3 (LMFE4)	NLMFE1 (NLMFE2)	NLMFE3 (NLMFE4)	NLMFE5 (NLMFE6)	NLMFE7 (NLMFE8)	NSSFE1 (NSSFE2)	NSSFE3 (NSSFE4)	NSSFE5 (NSSFE6)
CBINIT	Number of transient leakage zones and nodes.		x (x)		x (x)					
GNINIT	Number of element sides and zones for nonlinear head-dependent (Cauchy-type) boundaries and number of nonlinear point sinks.						x (x)			x (x)
INITB	Simulation title, number of: elements, nodes, time steps, stress periods, number of stress periods, zones, point sources or sinks, Cauchy-type boundaries, and specified-head nodes, maximum condensed bandwidth, and reduced-matrix bandwidth.	x	x	x	x	x	x	x	x	x
INITCG	Same as INITB except replace reduced-matrix bandwidth with maximum number of iterations and closure tolerance for MICCG solution method.	(x)	(x)	(x)	(x)	(x)	(x)	(x)	(x)	(x)
SWINIT	Number of water-table iterations, closure tolerance and maximum allowable displacement for for water-table iterations.							x (x)	x (x)	x (x)
VNINIT	Number of nonlinear steady vertical leakage zones.					x (x)			x (x)	

leakage flux from the previous time step, which is expressed by equations (179) and (181) in Cooley (1992), written for time-step n. Actually, the n+1 time level in these equations becomes the n level as the time step is incremented during simulation. Terms for the series contained in equation (201) in Cooley (1992) are computed and stored by node as the program vector CBTQ. The CBTQ vector also is used to store terms for the expression $Q_{Hi,n} + C_{Hi,n+1}[H_{i,n+1}/\Delta t_{n+1}]$ contained in equation (206) in Cooley (1992) for each node i. Two storage locations in CBTQ for each node are required for these terms and three storage locations are required for the series contained in equation (201) in Cooley (1992); thus, five storage locations are allocated for each node to store terms in the vector CBTQ. All terms just described are combined according to equation (206) in Cooley (1992) and are stored by node in the program vector CBQ. These terms represent components of the B vector of equation (1).

The steady vertical-leakage term associated with the transient leakage flux, C_{Ri}, given by equation (204) in Cooley (1992), is not formed by the "CB" subroutines which are added to the program structure of MODFE to simulate transient leakage. Terms that represent steady vertical leakage are computed as described in the previous section and are assembled into finite-element matrix equation (254) in Cooley (1992) for transient leakage.

Assembly of the transient-leakage terms into the finite-element matrix equation occurs in subroutine CBADEQ. The A vector, described in previous sections, is reused for the equation formation. Details about the reuse of computer storage and the equation formation are described in the section "Allocation of Computer Storage and Processing Time." The A-matrix term for transient leakage, $C_H(L)$, for node L, is added to the location in the A vector that corresponds to the main diagonal of the A matrix in equation (254) in Cooley (1992). This location is identified in subroutine CBADEQ as A(NME) for node L. The CBQ terms are added to the program vector B at location B(K), which stores the right side of the matrix equation for node L.

After computed heads are obtained for the time step, the part of the leakage flux associated with head changes is computed in subroutine CBTQC. From equation (198) in Cooley (1992), the new component of transient leakage, $\{[h_{i,n+1} - h_{i,n}]/\Delta t_{n+1}\gamma_i\}M_1[\gamma_i\Delta t_{n+1}]$ for node i and advanced time step n+1, is added to the old fluxes. The new flux is an approximation of $I_{mi,n+1}$, given by equation (179) in Cooley (1992), and is stored in the first three of five locations allocated to each node in program vector CBTQ. As the time-step index is incremented, these terms actually define $I_{mi,n}$, given in equations (178) in Cooley (1992), which are stored in program vector QOM1 in subroutine CBFMEQ. These terms are used for computing the P terms for the following time step, as described previously.

Table 6.—Subroutines that set dimensions, allocate storage, and initialize variables

Subroutine	Description of computations	Versions of MODFE that require subroutine								
		LMFE1 (LMFE2)	LMFE3 (LMFE4)	NLMFE1 (NLMFE2)	NLMFE3 (NLMFE4)	NLMFE5 (NLMFE6)	NLMFE7 (NLMFE8)	NSSFE1 (NSSFE2)	NSSFE3 (NSSFE4)	NSSFE5 (NSSFE6)
CBINIT	Allocate storage for transient leakage terms and initialize storage locations to zero.		x (x)		x (x)					
GNINIT	Allocate storage for α coefficients, node numbers, and controlling heads and altitudes for nonlinear head-dependent (Cauchy-type) boundaries and nonlinear point sinks. Initialize storage locations to zero.						x (x)			x (x)
INITB	Set dimensions for storage vectors, allocate storage for condensed matrix, reduced matrix, element areas and incidences, nodal coordinates, known fluxes, hydraulic head, boundary or external head, α coefficient, specified flux, boundary-node numbers, source-bed head, boundary-condition zone numbers, time steps, and node-indicator vector. Initialize time and flow-balance terms and storage locations for above terms to zero.	x	x	x	x	x	x	x	x	x
INITCG	Same as INITB, and allocate storage for vectors X, P, and R for MICCG method.	(x)	(x)	(x)	(x)	(x)	(x)	(x)	(x)	(x)
SWINIT	Allocate storage for aquifer thickness and altitude of top of aquifer, and initialize storage locations to zero.							x (x)	x (x)	x (x)
VNINIT	Allocate storage for hydraulic conductance term and altitudes for nonlinear steady vertical leakage. Initialize storage locations to zero.					x (x)			x (x)	
WTINIT	Allocate storage for head-change vector, aquifer thickness, altitude of top of aquifer, and specific yield for water-table simulations. Initialize storage locations to zero.			x (x)	x (x)	x (x)	x (x)	x (x)	x (x)	x (x)

Areally Distributed Sources and Sinks

The term for areally distributed sources and sinks expressed as $(1/3)W^e\Delta^e$ in equation (50) in Cooley (1992) for element e is computed in subroutine FMCO. This term represents the element contribution to the areally distributed flux at a node, which is part of the B vector of equations (1) and (2). Values for the volumetric flow rate per unit area [length/time], or the unit rate, are input by hydraulic-property zone as the program variable QD. The element contribution to areally distributed recharge or discharge expressed in equation (50) in Cooley (1992) is formed by computations similar to those performed for the storage-coefficient term: the unit rate is multiplied by the square of the scaling factor SCALE, divided by 6, and multiplied by twice the element area (program variable AREA see section "Storage Coefficient"). The resulting term is represented by program variable TEQ, and is added to the B vector of equations (1) and (2) for each node in the element. The B vector is represented by program vector Q. These computations are performed for all elements in the hydraulic-property zone and for all zones, thus satisfying the summation of areally distributed terms over all elements, as indicated by equation (50) in Cooley (1992).

The TEQ terms are summed in subroutine FMCO according to sign—positive for recharge—to obtain the terms used in the water-balance summary for areally distributed sources and sinks. It is convenient to perform the summation of TEQ terms at this location in MODFE as these terms are no longer needed after they are added into storage locations in the Q vector. The terms used in the water-balance summary for areally distributed sources and sinks are represented by DQI for recharge and DQO for discharge.

Point Sources and Sinks

Computations for incorporating point sources and sinks into matrix equations (1) and (2) are performed in subroutine DATIN. The volumetric rate [length^3/