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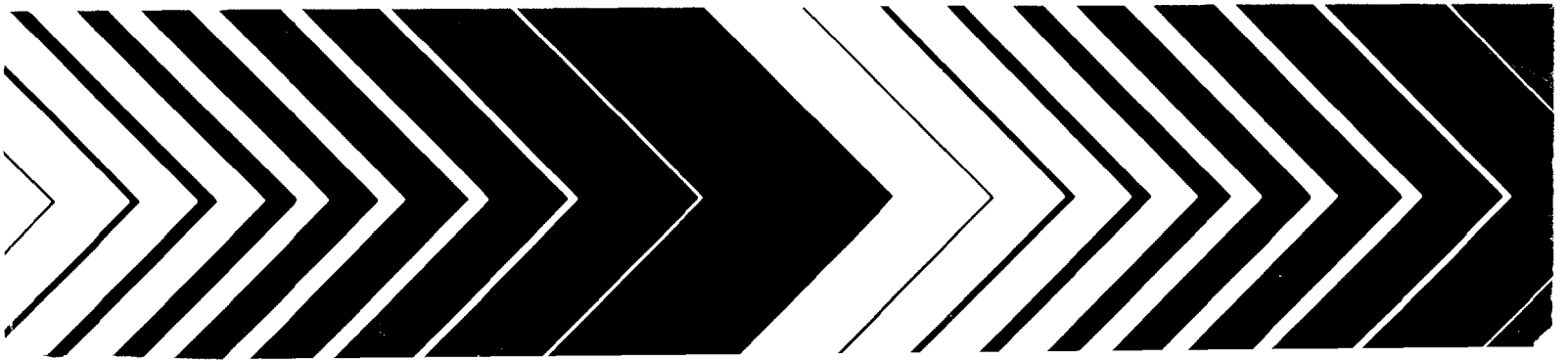
3DFEMWATER/ 3DLEWASTE: Numerical Codes for Delineating Wellhead Protection Areas in Agricultural Regions Based on the Assimilative Capacity Criterion



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3DFEMWATER/3DLEWASTE: NUMERICAL CODES FOR DELINEATING WELLHEAD PROTECTION AREAS IN AGRICULTURAL REGIONS BASED ON THE ASSIMILATIVE CAPACITY CRITERION

by

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FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient analytical tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Assessment Branch is developing management or engineering tools that can be used by States to protect public drinking water wells from possible contamination.

The 1986 Amendments to the Safe Drinking Water Act require each State to develop and submit to the U.S. EPA a wellhead protection program. As part of the program, States must establish procedures for delineating wellhead protection areas around each water well or well field which supplies a public water system. In order to delineate wellhead protection areas in agricultural regions using the assimilative capacity criterion, the 3DFEMWATER/3DLEWASTE model has been developed. These finite element numerical codes simulate 1) flow and transport in three-dimensional variably-saturated porous media under transient conditions, 2) multiple distributed and point sources/sinks, and 3) processes which retard the transport of contaminants.

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ABSTRACT

The 1986 Amendments to the Safe Drinking Water Act require each State to develop and submit to the U.S. EPA a wellhead protection program. As part of the program, States must establish procedures for delineating wellhead protection areas around each water well or well field which supplies a public water system. Of the five criteria that have been suggested by the U.S. EPA for delineating wellhead protection areas, the assimilative capacity criterion is potentially the most accurate. It takes into account the reduction in concentration of contaminants being transported toward a well caused by chemical and environmental processes at the land surface and in the vadose and saturated zones.

Nationwide, agricultural areas are located in many diverse hydrogeologic environments. Recharge and pumping rates can vary widely within an area because of irrigation practices and/or climate. In addition, contamination scenarios must consider multiple point and nonpoint source loadings of pesticides which vary both spatially and temporally. In order to delineate wellhead protection areas in agricultural regions using the assimilative capacity criterion, the use of a numerical model is needed that accounts for 1) flow and transport in three-dimensional variably-saturated porous media under transient conditions, 2) multiple distributed and point sources/sinks, and 3) processes which retard the transport of contaminants.

This document describes two related numerical codes, 3DFEMWATER and 3DLEWASTE, which can be used to delineate wellhead protection areas in agricultural regions using the assimilative capacity criterion. 3DFEMWATER (Three-dimensional Finite Element Model of Water Flow Through Saturated-Unsaturated Media) simulates subsurface flows, whereas 3DLEWASTE (Hybrid Three-Dimensional Lagrangian-Eulerian Finite Element Model of Waste Transport Through Saturated-Unsaturated Media) Models contaminant transport. Both codes treat heterogeneous and anisotropic media consisting of as many geologic formations as desired, consider both distributed and point sources/sinks that are spatially and temporally dependent, and accept four types of boundary conditions (i.e., Dirichlet (fixed-head or concentration), specified-flux, Neumann (specified-pressure-head gradient or specified-dispersive flux), and variable). The variable boundary condition in 3DFEMWATER simulates evaporation/infiltration/seepage at the soil-air interface and, in 3DLEWASTE, simulates mass infiltration into or advection out of the system. 3DLEWASTE contains options to model adsorption using a linear, Freundlich, or Langmuir isotherm, plus dispersion, and first-order decay.

This report was submitted in partial fulfillment of Work Assignment Number 1, Contract Number 68-CO-0019 by AQUA TERRA Consultants, under the sponsorship of the U.S. Environmental Protection Agency. This report covers the period May 1991 to July 1992, and work was completed as of August 1992.

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The 3DFEMWATER/3DLEWASTE code was developed by G.T. (George) Yeh of The Pennsylvania State University. Robert Strobl, also at The Pennsylvania State University, upgraded the code to meet U.S. Environmental Protection Agency coding conventions. John Kittle at AQUA TERRA Consultants reviewed the code and suggested modifications.

The original documentation of the 3DFEMWATER/3DLEWASTE code was prepared by G.T. Yeh. That documentation was substantially expanded and rewritten during the course of this project. At AQUA TERRA Consultants, Susan Sharp-Hansen was responsible for rewriting the documentation. She was assisted by Barry Lester of GeoTrans, Inc., who wrote Section 2 and part of the introduction; by Robert Strobl, who prepared some of the tables in the appendices; and by Jeff Scarborough of AScI Corporation, who applied the code to the example problems. John Imhoff, the Project Manager, supplied administrative guidance and he, Anthony Donigian, and John Kittle reviewed the document. Technical reviewers also included David Ward and Jeff Benegar of GeoTrans, Inc. Word processing was performed by Dorothy Inahara.

SECTION 1

INTRODUCTION

This document describes two related numerical codes, 3DFEMWATER and 3DLEWASTE. Together these codes can model flow and transport in three-dimensional variably-saturated porous media under transient conditions, with multiple distributed and point sources/sinks, and considering processes which retard the transport of contaminants (i.e., dispersion, decay and adsorption). Thus, they can be used to apply the assimilative capacity criterion to the development of wellhead protection areas. Background information about wellhead protection area delineation criteria and methods is provided in Section 1.1. The features and implementation of the 3DFEMWATER/3DLEWASTE codes are discussed in Section 1.2 and the contents of this document are summarized in Section 1.3.

It is important to note that the version of 3DFEMWATER/3DLEWASTE documented in this user's manual has **substantial CPU time requirements.** A faster version of the model is currently being developed.

1.1 WELLHEAD PROTECTION AREA DELINATION

The 1986 Amendments to the Safe Drinking Water Act require each State to develop and submit to the U.S. EPA a wellhead protection program. As part of the program, States must establish procedures for delineating wellhead protection areas around each water well or well field which supplies a public water system. A wellhead protection area (WHPA) is defined as the surface and subsurface area surrounding a water well or well field through which contaminants are likely to be transported and reach the well or wellfield. Within the WHPA, contaminant sources need to be assessed and managed to prevent pollution of public drinking water supplies. Existing WHP programs are generally aimed at one of the following overall protection goals:

- Provide a remedial action zone to protect wells from unexpected contaminant releases.
- Provide an attenuation zone to bring concentrations of specific contaminants to desired levels at the time they reach the wellhead.
- Provide a well-field management zone in all or part of a well's present or future recharge area.

Five criteria have been suggested by the U.S. EPA (U.S. EPA, 1987) for delineating wellhead protection areas that will adequately protect public water supplies. The criteria are:

- Distance, which considers a radial distance from the pumping well.

- **Drawdown,** which considers an area within which an aquifer's potentiometric surface has been lowered by pumping.

- **Time of travel,** which considers the time required for a contaminant to move through the subsurface to a well (often only considering advection).

- **Flow system boundaries,** which consider the geographic or hydrologic features that control groundwater flow.

- **Assimilative capacity,** which considers environmental factors which reduce the concentration of contaminants transported to a well.

One or more of the criteria may be used. The most technically demanding, but also potentially the most accurate, is the assimilative capacity criterion. The assimilative capacity criterion takes into account the reduction in concentration of contaminants being transported toward a well caused by chemical and environmental processes at the land surface and in the vadose and saturated zones.

The U.S. EPA has described six methods for applying the criteria to the delineation of WHPAs. Listed in order of difficulty, the methods are:

Arbitrary fixed radius, which involves drawing a circle around a well. The radius of the circle can be based on professional judgment or an established distance criterion.

- **Calculated fixed radius,** in which the radius of a circle around the well is determined from an equation that considers the volume of water pumped from a well over a specified time.

- **Simplified variable shapes,** which makes use of "standardized forms" representing various hydrogeologic and pumping conditions. The set of standardized forms are initially prepared using an analytical model. Subsequent application involves selecting the most appropriate shape for a given well.

- **Analytical methods,** which involve the application of analytical groundwater flow and transport models.

- **Hydrogeologic mapping,** which makes use of geologic, geophysical, and dye tracing techniques to map a WHPA.

- **Numerical models,** which involve the application of numerical models of flow and solute transport in the subsurface.

Application of the first three methods is suitable for only a very limited number of sites, such as extensive, homogeneous, single aquifers with a relatively flat potentiometric surface. While analytical methods are usually more technically accurate than the first three methods, their application is still restricted to relatively simple hydrogeologic environments. Hydrogeologic mapping may be the only reasonable method under some hydrogeologic conditions, such as karst or fractured aquifers. However, it will also be

necessary for some hydrogeologic mapping to be performed for application of either analytical or numerical models.

Numerical models provide the greatest flexibility and accuracy in representing complex environments and can be applied to nearly all types of hydrogeologic settings. The models can also be used to predict the dynamic aspects of the WHPA, such as changes in the size of the WHPA resulting from natural or man-made effects. Disadvantages for this method include costs that are high relative to other methods and the need for considerable technical expertise in hydrogeology and modeling. The cost may be warranted in areas where a high degree of accuracy is desired, however. Also, due to limitations on model grid spacing and density, numerical models are sometimes less suitable than analytical methods for assessing drawdowns close to pumping wells.

The more rigorous the method used for WHPA delineation, the smaller the WHPA can be without risking underprotection and the associated potential for water quality degradation. When a smaller WHPA can be defined without generating unacceptable risk, land use restrictions can be kept to a minimum along with the potential economic hardships associated with such land use restrictions. The choice of WHPA delineation methodology becomes a decision based on generating an acceptable margin of safety, while balancing the economic hardships to affected parties with the technical and economic feasibility of minimizing the WHPA.

1.1.1 Issues Related to Agricultural Regions

Nationwide, agricultural areas are located in many diverse hydrogeologic environments (e.g., multiple aquifer systems, fractured and/or karst systems, and systems with wide variations in depth to the water table). In addition, recharge can vary widely because of irrigation practices and/or climate. Also, domestic and irrigation wells, which pump at different and varying rates, are commonly located throughout agricultural regions. Therefore, the ability to model transient flow conditions (i.e., transient recharge, a fluctuating water table, and transient pumping from a variety of points in x,y,z space) for a wide variety of hydrogeologic conditions is important.

Contamination scenarios in agricultural regions must consider multiple point and nonpoint source loadings that vary both spatially and temporally. For example, spills, leaks, or the direct introduction of chemicals into well casings can result in point sources of contamination, whereas chemical application to fields can result in nonpoint sources of contamination.

Pesticide loadings to the subsurface are affected by both surface processes and agricultural management practices. Examples include runoff, erosion, chemical volatilization, evapotranspiration, tillage practices, and the method, amount, and timing of pesticide application. Most of these processes require detailed modeling of the surface environment or zone and are not addressed in models of subsurface flow and transport. Therefore, it is suggested that text or matrix ranking or the separate application of an existing model be used to estimate recharge and solute loading from the surface zone to the subsurface (e.g., PRZM-2, see Mullins et al., 1992).

The contaminants of concern in agricultural regions are predominantly organic pesticides and nitrates. Pesticides are typically present in the subsurface in dilute

concentrations. Because interest in agricultural areas is likely to focus on dilute organic pesticides, issues such as the transport of metals, the interactions of complex mixtures, or immiscible flow are not addressed by this model. Also, because of the complexity of the processes associated with the transport of nitrates, nitrate contamination can not be adequately modeled using this version of 3DFEMWATER/3DLEWASTE.

1.2 THE 3DFEMWATER/3DLEWASTE WHPA MODEL

3DFEMWATER (Three-dimensional Finite Element Model of Water Flow Through Saturated-Unsaturated Media) can be used to investigate subsurface flows as a stand-alone model, or it can be used to provide the hydrologic flow variables required by 3DLEWASTE. The special features of 3DFEMWATER are its flexibility and versatility in modeling a wide range of real-world problems. The model is designed to:

- Treat heterogeneous and anisotropic media consisting of as many geologic formations as desired.
- Consider both distributed and point sources/sinks that are spatially and temporally dependent.
- Accept prescribed initial conditions or obtain them by simulating a steady-state version of the system under consideration.
- Deal with a transient head variation over a freed-head (Dirichlet) boundary.
- Handle time-dependent fluxes due to a varying pressure gradient along a specified-pressure-head gradient (Neumann) boundary.
- Treat time-dependent total fluxes distributed over a specified-flux (Cauchy) boundary.
- Automatically determine variable boundary conditions of evaporation, infiltration, or seepage at the soil-air interface.
- Include the off-diagonal hydraulic conductivity components in the modified Richard's equation in order to deal with cases when the coordinate system does not coincide with the principal directions of the hydraulic conductivity tensor.
- Provide three options (exact, under-, and over-relaxation) for estimating the nonlinear matrix.
- Include two options (successive subregion block iterations and successive point iterations) for solving the linearized matrix equations.
- Automatically reset the time-step size when boundary conditions or sources/sinks change abruptly.

3DLEWASTE (Hybrid Three-Dimensional Lagrangian-Eulerian Finite Element Model of Waste Transport Through Saturated-Unsaturated Media) uses a hybrid Lagrangian-Eulerian approach. In comparison to conventional finite element (including both

Galerkin and upstream finite element) or finite difference (including both central and upstream finite difference) models, 3DLEWASTE offers several advantages. First, it completely eliminates numerical oscillation due to advection terms. Second, it can be applied to mesh Peclet numbers ranging from zero to infinity. (Conventional finite element or finite difference models typically impose severe restrictions on the mesh Peclet number.) Third, it can use very large time-step sizes to greatly reduce numerical dispersion. In fact, the larger the time step, the better is the solution with respect to advective transport. The time-step size is only limited by the accuracy requirement with respect to diffusive/dispersive transport, which is normally not a very severe restriction. Finally, the hybrid Lagrangian-Eulerian finite element approach is always superior to, and will never be worse than, its corresponding upstream finite element method.

The 3DLEWASTE model is designed to:

- Treat heterogeneous and anisotropic media.
- Consider spatial and temporal distribution, as well as point sources/sinks.
- Accept prescribed initial conditions or obtain them by simulating a steady-state version of the system under consideration.
- Deal with transient concentrations distributed over prescribed concentration (Dirichlet) boundaries.
- Handle time-dependent fluxes over variable boundaries.
- Deal with time-dependent total fluxes over specified-flux (Cauchy) boundaries.
- Handle time-dependent fluxes over specified dispersive-flux (Neumann) boundaries.
- Include the off-diagonal dispersion coefficient tensor components in the governing equation for dealing with cases when the coordinate system does not coincide with the principal directions of the dispersion coefficient tensor.
- Provide two options of treating the mass matrix--consistent and lumping.
- Provide three options (exact, under- and over-relaxation) for estimating the nonlinear matrix.
- Include a block iteration method to solve the linearized matrix equations to eliminate the excessive storage demands of a direct band matrix solution.
- Automatically reset the time-step size when boundary conditions or sources/sinks change abruptly.
- Simulate first-order contaminant decay.
- Include three adsorption models--a linear isotherm and a nonlinear Freundlich or Langmuir isotherm.

1.2.1 Experience Required to Apply 3DFEMWATER/3DLEWASTE

The complexity and sophistication of the 3DFEMWATER/3DLEWASTE numerical codes limits the number of people who can successfully use the codes to apply the assimilative capacity criterion in wellhead protection area delineation. The user community is expected to be State personnel, as well as personnel at the U.S. EPA headquarters and regional offices, who are experienced numerical modelers with a strong background in hydrogeology.

1.2.2 Implementing a 3DFEMWATER/3DLEWASTE Modeling Study

Implementation of a 3DFEMWATER/3DLEWASTE modeling study represents a highly rigorous evaluation of a wellhead site. The study is generally aimed at delineating the WHPA with a high degree of certainty. The project team can take into consideration the specific nature of present and future wellfields, the physical and chemical nature of potential contaminant sources, the effect of human activities, as well as the complexity of the groundwater flow system through which the contaminants travel.

Although 3DFEMWATER/3DLEWASTE studies can provide flexibility in defining the hydrogeologic environment and contaminant sources, they are limited by the quantity and quality of physical and chemical data available to define the system. When seeking to define the zone of contribution in a WHPA using a 3DFEMWATER/3DLEWASTE analysis, there is a law of diminishing returns. The economic benefits gained from being able to minimize land use restrictions must be weighed against the costs of generating the necessary data and applying the model.

Wellfield geometry and the spatial distribution of wells within a field can strongly affect subsurface flow at regional and local scales. Using the 3DFEMWATER/3DLEWASTE model, an investigator can consider the influence of a wellfield on the regional flow system. On the local scale, the effects of partial penetration associated with well screening intervals can also be considered. Localized flow patterns, which result from perturbations to the flow field and the heterogeneous nature of the geologic medium, influence the movement of dissolved contaminants and determine 1) the amount of time required for a dissolved species to reach the wellfield and 2) the degree of attenuation of the species as it approaches the field.

The 3DFEMWATER/3DLEWASTE model also allows the user to examine the influence of temporal changes in well production on contaminant mobility. The influence of seasonal variations in well production and other periodic variations (i.e., drought conditions, unseasonably warm summers, etc.), can strongly affect the potential for a contaminant to reach a wellfield at unacceptable levels or in an unacceptable amount of time. The temporal variations in well production can be considered in conjunction with associated temporal changes in recharge and evapotranspiration rates.

As implied above, the 3DFEMWATER/3DLEWASTE model is not limited to discretization of the flow field into regularly shaped prismatic blocks (i.e. triangular and rectangular prisms). Therefore, consideration of the heterogeneous nature of a modeled system is mainly limited by either the availability of data or the computational power of the computer utilized. There is a practical limitation on the degree of heterogeneity which can be simulated, based on the conflict between the grid block-size restrictions

needed to circumvent convergence problems and the number of blocks that a computer can handle in a time-efficient manner. Within these restrictions, it is the model user's goal to maximize the extent to which the influence of soil and rock-type heterogeneities affect the flow system.

In nature, heterogeneities generate a strong control on the local pathways that the dissolved chemicals will follow. The tendency for water to flow through low resistance (high conductivity) pathways provides a short-circuiting effect that can accelerate the movement of chemicals to a wellfield. In contrast, occurrences of high resistance (low conductivity) media between the source and the screened intervals of wells can inhibit the contaminant from reaching the water supply or attenuate the contaminant to safe concentration levels before it reaches the water supply. The uncertainty associated with a WHPA analysis is directly related to the presence of heterogeneity in the aquifer properties. As the degree of heterogeneity decreases, the possibility of underestimating or overestimating the chemical migration is reduced. On the other hand, the potential for contamination is most uncertain when using bulk properties or using ***ad hoc*** variances in the values of effective porosity, dispersivity and hydraulic conductivity.

Since the flow portion of 3DFEMWATER/3DLEWASTE simulates variably-saturated conditions, a more accurate model of water storage in unconfined or partially confined systems can be generated. The user can consider draining (and filling) of pore spaces above the water table, which can damp the effect of time-variant changes in well production, recharge and evapotranspiration on the flow system. Rigorous representation of the unsaturated zone also permits examination of the influence of variable saturation on the mobility of contaminants. Vertical infiltration through the unsaturated zone and the associated lateral spreading of contaminants, due to the occurrence of sediment lenses of various grain sizes, can be considered. Explicit simulation of the unsaturated zone also allows for direct consideration of the contaminant storage capacity of the unsaturated zone. This more accurately depicts the role of the unsaturated zone as a source of contaminant infiltration into the saturated zone. The availability of different adsorption models (linear, Freundlich and Langmuir) allows the user to choose a contaminant storage capacity appropriate for the waste being modeled.

The 3DFEMWATER/3DLEWASTE model includes a relatively rigorous representation of contaminant sources by using a variety of time-dependent boundary conditions. Contaminant sources may be represented not only as point sources or sources of simple geometry, as assumed in analytical solutions, but also as sources of variable geometry. Where applicable, contaminants already present in the subsurface water and solid matrix at the start of a modeling study can also be simulated. The use of infiltration or recharge options available in the 3DFEMWATER/3DLEWASTE model provides a good method of simulating contaminant sources such as spatially- and temporally-variant pesticide or fertilizer applications to agricultural areas.

The interaction of the regional flow field and local wellfield perturbations can be handled in two ways using 3DFEMWATER/3DLEWASTE. The localized flow field may be implemented as a freely discretized portion of the larger system where the boundary conditions are generally associated with the regional flow field. The problem can also be broken up into two problems of different scales, where the regional flow system is modeled for flow only and the local system is modeled for flow and transport with the boundary conditions generated from the regional flow model. The degree of interaction

between the two models is dictated by the degree of accuracy desired, and the placement of local system boundaries.

1.3 ORGANIZATION OF THE DOCUMENT

This documentation contains the information needed to understand and apply the 3DFEMWATER/3DLEWASTE codes to wellhead protection area delineation problems. Section 2 contains information on model distribution and support. In Section 3, background related to the model equations, features, and numerical approximation techniques is presented. Section 4 is a guide to the construction of input data sets for the code. Assistance in explaining and estimating some of the input parameters is provided in Section 5. Five simple example problems, including the corresponding input data files, are given in Section 6. The appendices contain more detailed information about the numerical codes, including descriptions of the subroutines, and listings of the maximum control parameters and program variables.

SECTION 2

MODEL DEVELOPMENT, DISTRIBUTION, AND SUPPORT

NOTE: Refer to the READ.ME file for the latest supplemental information, changes, and/or additions to the 3DFEMWATER/3DLEWASTE model documentation. A copy of the READ.ME file is included on each distribution diskette set or it can be downloaded from the Center for Exposure Assessment Modeling (CEAM) electronic bulletin board system (BBS). It can be installed on a hard disk using the INSTALL (diskette) or INSTALPZ (BBS) program. It is an ASCII (non-binary) text file that can be displayed on the monitor screen by using the DOS TYPE command (e.g., TYPE READ. ME) or printed using the DOS PRINT command (e.g., PRINT READ.ME).

The READ.ME file contains a section entitled File Name and Content that provides a brief functional description of each 3DFEMWATER/3DLEWASTE file by name or file name extension type. Other sections in this document contain further information about:

- System development tools used to build the microcomputer release of the 3DFEMWATER/3DLEWASTE model.
- Recommended hardware and software configuration for execution of the model and all support programs.
- Program execution.
- Minimum file configuration.
- Sample run times.
- Program modification.
- Technical support.

2.1 DEVELOPMENT AND TESTING

The 3DFEMWATER/3DLEWASTE model was developed and tested on a Digital Equipment Corporation (DEC) VAX6310 running under version 5.4-2 of the VMS operating system (OS) and version 5.5-98 of VAX VMS FORTRAN- 77, and an Advanced Logic Research (ALR) 486/25 microcomputer running under version 4.00 of IBM PC DOS and version 2.51 of Salford FORTRAN (FTN77/486). The following FORTRAN tools were also used to perform static evaluations of the 3DFEMWATER/3DLEWASTE FORTRAN code on an IBM PS/2 Model 80-071 running under version 3.3 of IBM PC! DOS, MICRO EXPRESS (ME) 486/25 and 486/33 systems running under version 5.00 of Microsoft (MS) DOS, and a Sun SPARCstation 1+GX running version 4.1.1 of UNIX/SunOS:

- Ryan-McFarland FORTRAN versions 2.45, 3.10.01 (RMFORT).
- Microsoft FORTRAN version 5.00 (MSFORT).
- Lahey FORTRAN versions 5.01, 4.02 (F77L, F77L-EM/32).
- Waterloo FORTRAN version 8.5E (WATCOM FORTRAN-77/386).
- Sun FORTRAN version 1.4.
- Silicon Valley FORTRAN version 2.81 (SVS FORTRAN-77/386).

In addition to the VAX and ALR systems, 3DFEMWATER/3DLEWASTE has also been successfully executed on a PRIME 50 Series minicomputer running under PRIMOS, the Sun SPARCstation, and the IBM PS/2 Model 80-071.

2.2 DISTRIBUTION

The 3DFEMWATER/3DLEWASTE model and all support files and programs are available on diskette from the Center for Exposure Assessment Modeling, located at the U.S. EPA Athens Environmental Research Laboratory, Athens, Georgia, at no charge. The CEAM has an exchange diskette policy. It is preferred that diskettes be received before sending a copy of the model system (refer to Section 2.3, Obtaining a Copy of the 3DFEMWATER/3DLEWASTE Model).

Included in a distribution diskette set are:

- 3DFEMWATER/3DLEWASTE general execution and user support guide (READ. ME) file.
- Interactive installation program (refer to Section 2.5).
- Test input and output files for installation verification.
- Executable task image file for the 3DFEMWATER/3DLEWASTE model.
- FORTRAN source code files.
- Command and/or “make” files to compile, link, and run the task image file (*. EXE).

A FORTRAN compiler and link editor are NOT required to execute any portion of the model. If the user wishes to modify the model, it will be up to the user to supply and/or obtain:

- An appropriate text editor that saves files in ASCII (non-binary) text format.
- FORTRAN development tools to recompile and link edit any portion of the model.

CEAM cannot support, maintain, and/or be responsible for modifications that change the function of the executable task image, MAKE, or DOS command files supplied with this model package.

The microcomputer release of the 3DFEMWATER/3DLEWASTE model is a full implementation of the VAX/VMS version. The microcomputer implementation of this model performs the same function as the U.S. EPA mainframe/minicomputer version.

2.3 OBTAINING A COPY OF THE 3DFEMWATER/3DLEWASTE MODEL

NOTE: The following abbreviations are used below to represent different quantities of computer memory:

1 k = 1 kilobyte = 1,024 bytes
1 m = 1 megabyte = 1 "meg" = 1,048,576 bytes
l b = l b y t e

2.3.1 Diskette

To obtain a copy of the 3DFEMWATER/3DLEWASTE distribution model package on diskette, send:

- The appropriate number of double-sided, double-density (DS/DD 360kb) 5.25 inch, or double-sided, high-density (DS/HD 1.44mb) 3.5 inch error-free diskettes.

  NOTE: To obtain the correct number of diskettes, contact CEAM at 706/546-3549.

- A cover letter, with a complete return address requesting the 3DFEMWATER/3DLEWASTE model to:

  Model Distribution Coordinator
  (ATTN: Catherine E. Green, CSC)
  Center for Exposure Assessment Modeling
  Environmental Research Laboratory
  U.S. Environmental Protection Agency
  Athens, GA 30613-0801

Program and/or user documentation, or instructions on how to order documentation, will accompany each response.

2.3.2 Electronic Bulletin Board System (BBS)

To download a copy of the 3DFEMWATER/3DLEWASTE model, or to check the status of the latest release of this model or any other CEAM software product, call the CEAM BBS 24 hours a day, 7 days a week. To access the BBS, a computer with a modem and communication software are needed. The phone number for the BBS is 706/546-3402. Communication parameters for the BBS are:

- 300/1200/2400/9600 baud rate.
- 8 data bits.
- No parity.
- 1 stop bit.

In order to access the BBS at 9600 baud, a USRobotics Courier HST modem must be used.

2.4 GENERAL/MINIMUM HARDWARE AND SOFTWARE INSTALLATION AND RUN TIME REQUIREMENTS

NOTE: Refer to the READ.ME file for the latest supplemental and more complete information, changes, and/or additions concerning specific hardware and software installation and run time requirements.

2.4.1 Installation Requirements

- 3.5 inch, 1.44mb diskette drive, or 5.25 inch, 360kb diskette drive.
- Hard disk drive.
- Approximately 8mb free hard disk storage,

2.4.2 Run Time Requirements

- 386 or 486 compatible microcomputer.
- MS or PC DOS version 3.30 or higher.
- 640k base memory.

Extended memory and hard disk storage requirements will vary with the size of the problem being simulated. Requirements for problems similar to those found in Section 6 are:

- 2mb of extended (XMS) memory.
- 4mb free hard disk storage.

Refer to READ.ME file for suggested modification of the CONFIG.SYS and/or AUTOEXEC.BAT DOS system configuration and start-up files.

2.5 INSTALLATION

To install the 3DFEMWATER/3DLEWASTE model and/or related support files on a hard disk, insert the first distribution diskette in a compatible diskette drive (refer to Section 2.4). Then type:

A:\INSTALL or B:\INSTALL

at the DOS system prompt and press the <Enter> key. Then follow instructions and respond to prompts presented on the monitor screen by the interactive installation program. Complete installation instructions are also printed on each external diskette label. The 3DFEMWATER/3DLEWASTE distribution diskette sets implement software product installation standards to insure the most error-free, maintainable, and user-acceptable distribution of CEAM products. It has a “unique menu option, command, full-screen (interactive), diagnostic, error-recovery, help, and selective installation capabilities using state-of-the-art human-factors engineering practices and principles.

NOTE: The contents of the distribution diskettes can be copied to another set of “backup” diskettes using the DOS DISKCOPY command. Refer to the DOS Reference Manual for command application and use. The “backup” diskettes must be the same size and storage density as the original, source diskettes.

2.6 INSTALLATION VERIFICATION AND ROUTINE EXECUTION

Refer to the following sections in the READ.ME file for complete instructions concerning installation verification and routine execution of the 3DFEMWATER/3DLEWASTE model:

- File name and content.
- Routine execution.
- Run time and performance.
- Minimum file configuration.

2.7 CODE MODIFICATION

Included in the diskette set are:

- An executable task image file for the 3DFEMWATER/3DLEWASTE model.
- FORTRAN source code files.
- Command and/or “make” files to compile, link, and run the task image file (*.EXE).

If the user wishes to modify the model or any other program, it will be up to the user to supply and/or obtain:

- An appropriate text editor that saves files in ASCII (non-binary) text format.
- FORTRAN development tools to recompile and link edit any portion of the model.

CEAM cannot support, maintain, and/or be responsible for modifications that change the function of any executable task image (*. EXE), DOS batch command (*. BAT), and/or "make" utility file(s) supplied with this model package.

2.8 TECHNICAL HELP

For questions and/or information concerning:

- Installation and/or testing of the 3DFEMWATER/3DLEWASTE model and/or support programs or files, call 706/546-3590, 3548 for assistance.

- 3DFEMWATER/3DLEWASTE model and/or program content, application, and/or theory, call 706/546-3 171 for assistance.

- Use of the CEAM electronic bulletin board system (BBS), contact the BBS system operator (SYSOP) at 706/546-3548.

- CEAM software and distribution Quality Assurance and Control, call 706/546-3634.

- Other environmental software and documentation distributed through CEAM, contact the Model Distribution Coordinator at 706/546-3549.

- Other support available through CEAM, contact Mr. Robert B. Ambrose, Jr., CEAM Manager:

  - By mail at the following address:

    Center for Exposure Assessment Modeling (CEAM)
    Environmental Research Laboratory
    U.S. Environmental Protection Agency
    Athens, Georgia 30613-0801

  - By telephone at 706/546-3130.

    By fax at 706/546-2018.

  - Through the CEAM BBS message menu and commands. The CEAM BBS communication parameters and telephone number are listed above.

2.8.1 Electronic Bulletin Board System (BBS)

To help technical staff provide better assistance, write down a response to the following topics before calling or writing. If calling, be at the computer, with the computer on, and in the proper sub-directory when the call is placed.

Program information:

Describe the problem, including the exact wording of any error and/or warning message(s).

List the exact steps, command(s), and/or keyboard key sequence that will reproduce the problem.

Machine information:

List computer brand and model.

- List available RAM (as reported by DOS CHKDSK command).
- List available extended memory (XMS).
- List name and version of extended memory (XMS) manager (i.e., HIMEM, VDISK, RAMDRIVE, etc.).
- List available hard disk space (as reported by DOS CHKDSK command).
- List the brand and version of DOS (as reported by DOS VER command).
- List the name of any memory resident program(s) installed.
- Printer brand and model.
- Monitor brand and model.

NOTE: If contacting CEAM by mail, fax, or BBS, include responses to the above information in your correspondence.

2.9 DISCLAIMER

Mention of trade names or use of commercial products does not constitute endorsement or recommendation for use by the United States Environmental Protection Agency.

Execution of the 3DFEMWATER/3DLEWASTE model, and modifications to the DOS system configuration files (i.e., /CONFIG.SYS and /AUTOEXEC.BAT) must be made at the user's own risk. Neither the U.S. EPA nor the program authors can assume responsibility for model and/or program modification, content, output, interpretation, or usage.

CEAM software products are built using FORTRAN-77, assembler, and operating system interface command languages. The code structure and logic of these products is designed for single-user, single-tasking, non-LAN environment and operating platform for microcomputer installations (i.e., single user on a dedicated system).

Users will be on their own if they attempt to install a CEAM product on a multi-user, multi-tasking, and/or LAN based system (i.e., Windows, DESQview, any LAN). CEAM

cannot provide installation, operation, and/or general user support under any combination of these configurations. Instructions and conditions for proper installation and testing are provided with the product in a READ.ME file. While multiuser/multitasking/LAN installations could work, none of the CEAM products have been thoroughly tested under all possible conditions. CEAM can provide scientific and/or application support for selected products if the user proves that a given product is installed and working correctly.

2.10 TRADEMARKS

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SECTION 3

BACKGROUND INFORMATION

3.1 3DFEMWATER

3DFEMWATER is designed to simulate the movement of moisture through variably-saturated porous media. Typical applications include: 1) studying the influence of transient stresses, such as well production schemes or the onset of drought conditions, on water table elevations, and 2) generating flow fields for use in examining the influence of physical processes such as rainfall and evapotranspiration on the movement of dissolved contaminants through the vadose zone and into aquifers (Figure 3.1). The complementary 3DLEWASTE model is designed to utilize the flow data generated by 3DFEMWATER simulations in order to evaluate the associated movement of dissolved contaminants through the modeled system. The model 3DLEWASTE is described in Section 3.3.

3.1.1 Governing Equations

The governing equation for flow of water through a variably-saturated porous medium, as derived from mass and momentum conservation constraints, can be written:

$$F(h)\frac{\partial h}{\partial t} = \nabla \cdot [K(h) \cdot (\nabla h + \nabla z)] + q \qquad (3\text{-}1)$$

where

h	=	pressure head (L)
z	=	distance above a datum (L)
$K(h)$	=	effective hydraulic conductivity (L/T)
$F(h)$	=	water (storage) capacity (1/L)
q	=	source/sink term ($L^3/T/L^3$)
t	=	time (T)
∇	=	gradient
$\nabla\cdot$	=	divergence

Equation 3-1, often referred to as Richard's equation, differs from the governing equation for saturated flow through porous media because of the nonlinearity of the hydraulic conductivity and storage terms. The effective hydraulic conductivity can be rewritten as the product of nonlinear and constant terms in the form:

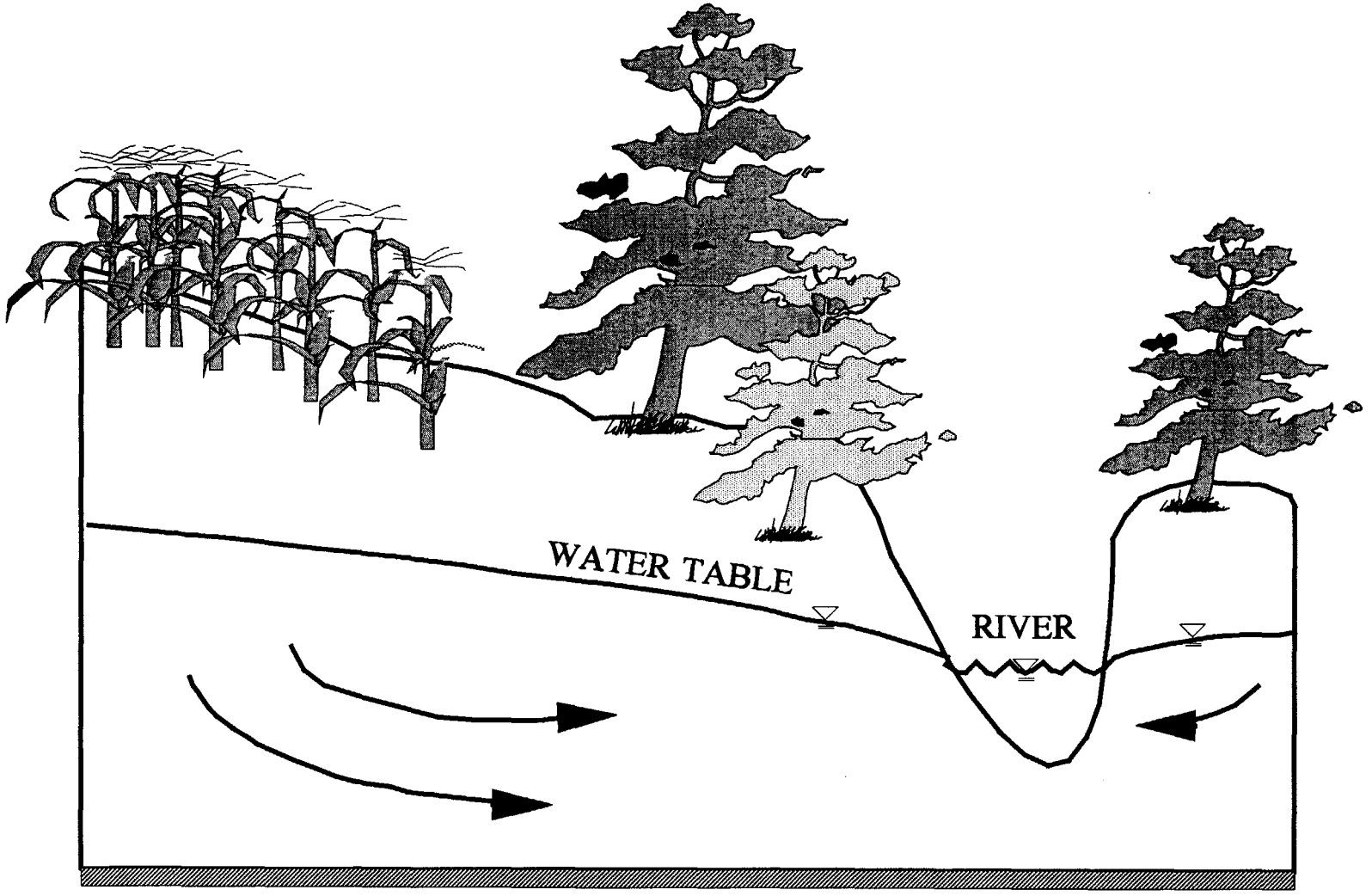


Figure 3.1 Unconfined aquifer to be approximated as a variably-saturated porous medium.

$$K(h) = k_r K_s \tag{3-2}$$

where k_r is the relative permeability, ranging in value from 0.0 to 1.0, and K_s is the saturated hydraulic conductivity (L/T). The saturated hydraulic conductivity is a flow property of both the porous medium and fluid, and is determined by tests performed under saturated conditions. It represents a maximum possible value of effective hydraulic conductivity. The relative permeability term describes the influence of water content on the magnitude of the effective hydraulic conductivity. Values of relative permeability range from a minimum value reflecting the reduction of effective conductivity at residual water content to a maximum of 1.0 reflecting saturated conditions.

The change in relative permeability is caused by changes in moisture content, resulting in the preferential movement of water through certain pathways, due to the influence of capillary forces. As the soil becomes less saturated, water drains more readily from the large radius pore structures, the water flow becomes restricted to pore sequences of smaller radii (Figure 3.2) as well as those held in layers close to the soil particles. The result of water becoming increasingly restricted to the smaller radius pathways is a reduction in the spatially-averaged effective hydraulic conductivity.

The decrease in effective hydraulic conductivity, as reflected in the relative permeability term, is described by pairs of empirical soil-moisture curves, These curves detail the relationships between water content and pressure head, and between hydraulic conductivity and water content. Soil-moisture curves are often described as coefficients and exponents of standard analytical functions (Brooks and Corey, 1966; Mualem, 1976; van Genuchten, 1980). The 3DFEMWATER code allows the user to define the curves using the van Genuchten functions (1980) or as sets of paired values of relative permeability versus moisture content and moisture content versus pressure head given in lookup table format. The van Genuchten relationships found in 3DFEMWATER are:

$$k_r = \theta_e^{1/2}\left[1 - \left(1 - \theta_e^{1/\gamma}\right)^{\gamma}\right]^2 \tag{3-3a}$$

and

$$\theta_e = \begin{cases} [1 + (\alpha|h-h_a|)^{\beta}]^{-\gamma} & \text{for } h<h_a \\ 1 & \text{for } h \geq h_a \end{cases} \tag{3-3b}$$

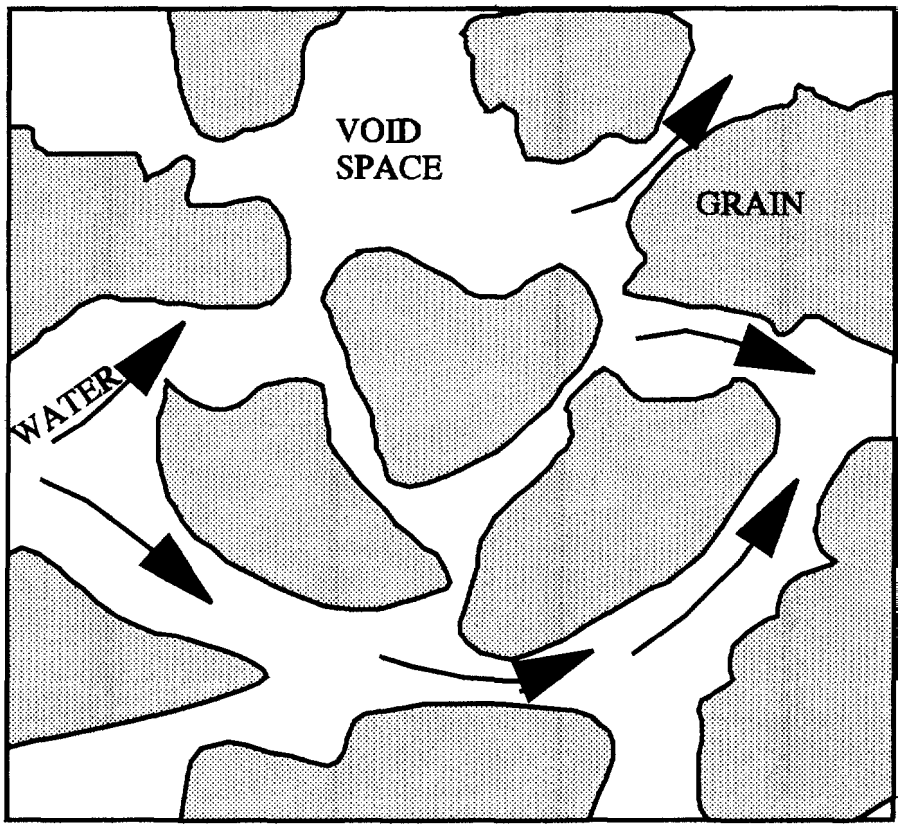


Figure 3.2. Variable pore spacing in soil under saturated flow conditions.

where

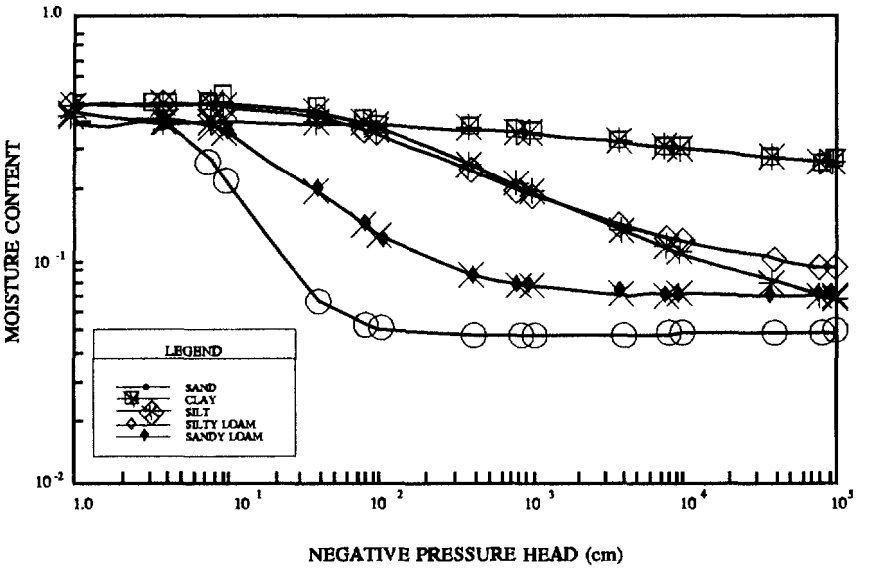
$$\theta_e = \frac{\theta_w - \theta_{wr}}{\phi - \theta_{wr}} \tag{3-3c}$$

$$\gamma = 1 - 1/\beta \tag{3-3d}$$

and

θ_w = moisture content (dimensionless)
ϕ = porosity (dimensionless)
θ_{wr} = residual moisture content (dimensionless)
β, γ = soil-specific exponents (dimensionless)
α = soil-specific coefficient (l/L)
h_a = air entry pressure head (L)
θ_e = effective moisture content (dimensionless)

Note that the soil-moisture content is defined as the porosity multiplied by the degree of saturation. Typical soil-moisture curves generated from Equations 3-3a and 3-3b are presented in Figures 3.3a and 3.3b.



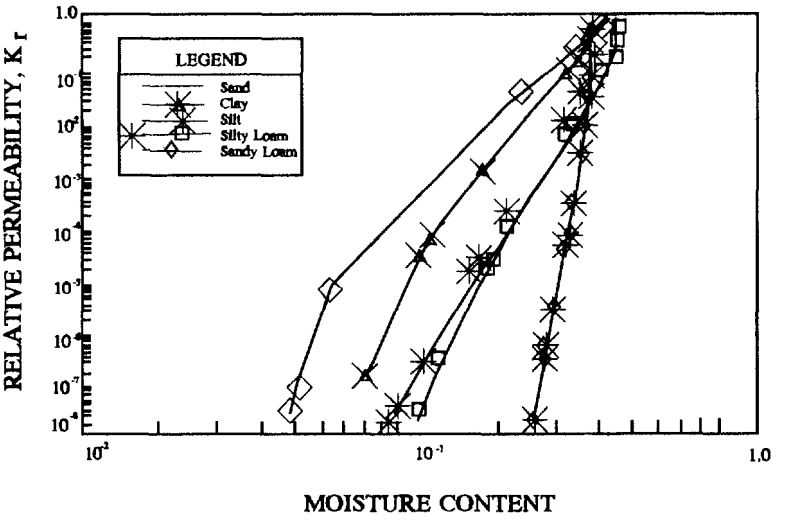


Figure 3.3. Logarithmic plot of constitutive relations for sand, clay, silty loam, and sandy loam: (a) moisture content vs. pressure head, and (b) relative permeability vs. moisture content (based on data presented in Carsel and Parrish, 1988).

The water capacity term or storage term used in 3DFEMWATER can be written in the form:

$$F(h) = d\theta_w/dh \tag{3-4}$$

It should be noted that, due to the relatively small influence of compressibility on water capacity in the unsaturated zone (with respect to the drainage potential), soil and water compressibility have been ignored in the storage term. When analytical functions are used to describe the nonlinearity of the relative conductivity, the derivative with respect to pressure head of the water content versus pressure head function must also be defined analytically.

The equation governing saturated flow represents a limiting case of Richard's equation where the relative permeability is a constant of 1.0 and the water capacity is a constant equal to the specific yield for an unconfined aquifer or specific storage for a confined aquifer.

3.1.2 Boundary Conditions and Transient Source/Sink Terms

Unique solutions to variably-saturated flow problems are generated by solving Richard's equation in conjunction with 1) a set of boundary conditions defined at the physical edges of the modeled system and 2) where appropriate, source/sink terms applied within the system (Figure 3.4). Boundary conditions available in the 3DFEMWATER model include fixed-head (Dirichlet) boundaries, specified-flux (Cauchy) boundaries, specified pressure-head gradient (Neumann) boundaries and variable (head-dependent flow) boundaries.

Fixed-head or *Dirichlet* boundaries are boundaries defined by prescribing pressure heads at specified boundary nodes so that:

$$h = h_d(x_b,y_b,z_b,t) \text{ on } B_d \tag{3-5}$$

where

h_d	= specified pressure head (L)
B_d	= portion of the system boundary subject to a Dirichlet boundary condition
x_b,y_b,z_b	= spatial coordinates on the boundary (L)

Dirichlet boundaries are typically used to define the perimeters of bodies of water, the water table location, and leaking surface impoundments or other waste disposal facilities containing specified levels of water. Specified pressure heads may be constant or allowed to vary with time reflecting physical processes such as water level fluctuations associated with seasonal changes in rainfall and evapotranspiration rates.

The *specified-flux (Cauchy)* boundary represents the portions of the system boundary where infiltration or evapotranspiration rates can be quantified. The specified-flux boundary condition can be written:

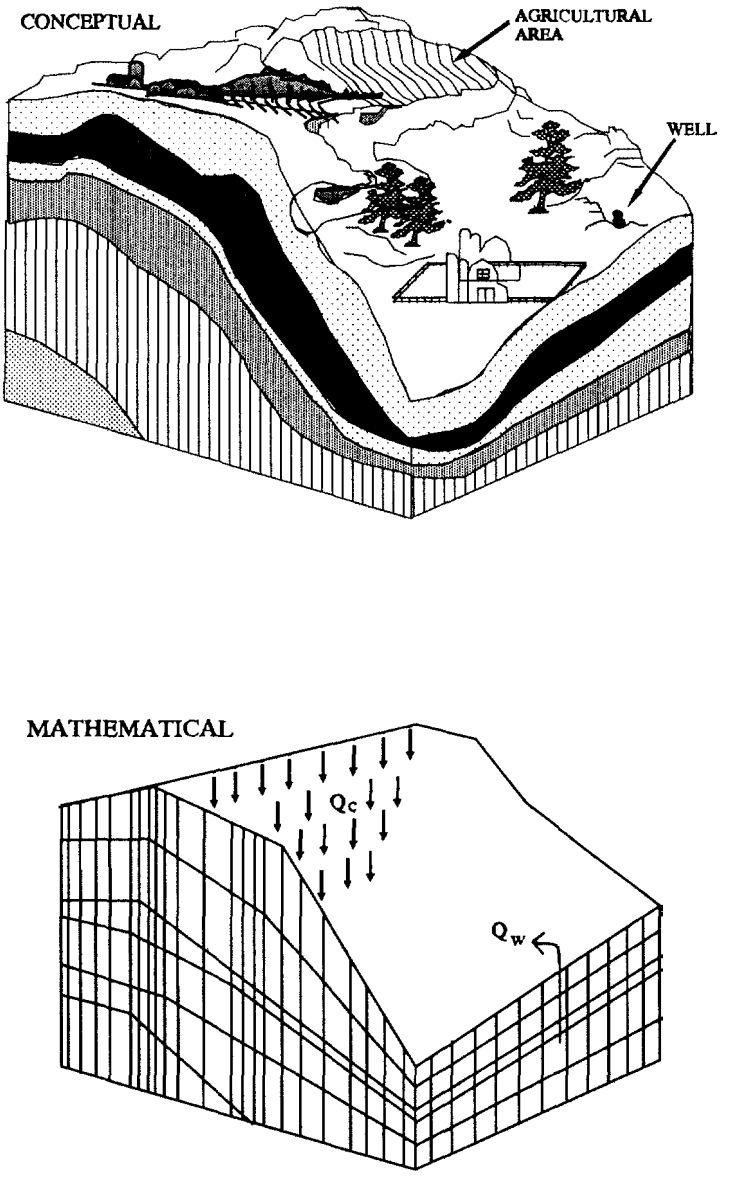


Figure 3.4. Conceptual model and mathematical approximation for a variably-saturated flow system. Within the modeled system, transient source/sink terms may be applied as point sources/sinks or as distributed sources/sinks.

$$-\mathbf{n}\cdot k_r K_s \cdot(\nabla h + \nabla z) = q_c(x_b,y_b,z_b,t) \text{ on } B_c \quad (3\text{-}6)$$

where

$\mathbf{n}$ = outward unit vector normal to the boundary
∇h = pressure head gradient
∇z = gravity gradient
q_c = specified flux rate (L/T)
B_c = portion of the system boundary subject to a specified-flux boundary condition
k_r = relative permeability
K_s = saturated hydraulic conductivity (L/T)

The specified-flux condition is analogous to a *Neumann* boundary condition for saturated flow problems differing only in the nonlinear nature of the effective hydraulic conductivity. The specified boundary is simulated by assigning water flux rates along specified element sides. Flux rate versus time profiles can be input to account for seasonal or other time-variant changes in rainfall and evapotranspiration rates. The default boundary condition for 3DFEMWATER is a zero specified-flux boundary condition, $q_c=0$.

Also available in 3DFEMWATER is a *specified-pressure-head gradient (Neumann)* boundary condition of the form:

$$-\mathbf{n}\cdot k_r K_s \cdot \nabla h = q_n(x_b,y_b,z_b,t) \text{ on } B_n \quad (3\text{-}7)$$

where q_n (L/T) is the portion of the boundary flux attributable to the pressure-head gradient and B_n is the portion of the system boundary subject to a specified-pressure-head gradient boundary condition. For unsaturated flow problems, the presence of this option provides the user an efficient way of evaluating systems with vertically extensive vadose zones, As long as the area of interest in a study is above the capillary fringe, the specified-pressure-head gradient boundary condition allows the user to truncate the system above the water table without knowing fluxes or pressure heads a priori (Figure 3.5). By choosing the specified-pressure-head gradient boundary condition option for element faces defining the bottom boundary of the system, and setting the flux q_n equal to zero, the bottom boundary becomes a gravity drainage boundary. This is equivalent to the code allowing the user to specify a flux along a horizontal bottom boundary of $q_c=k_r K_s$. This assumption of zero vertical change in pressure head near the bottom boundary is a reasonable assumption for slowly varying flow conditions and represents the outflow boundary condition that is usually assumed for field drainage experiments. This boundary condition is not appropriate for use in modeling the saturated zone.

The *variable composite* boundary condition represents a combined Dirichlet/specified-flux boundary. It allows for time-variant infiltration/evapotranspiration rates with limits set on the maximum and minimum pressure heads which the boundary nodes may attain. The variable boundary conditions during periods of precipitation are:

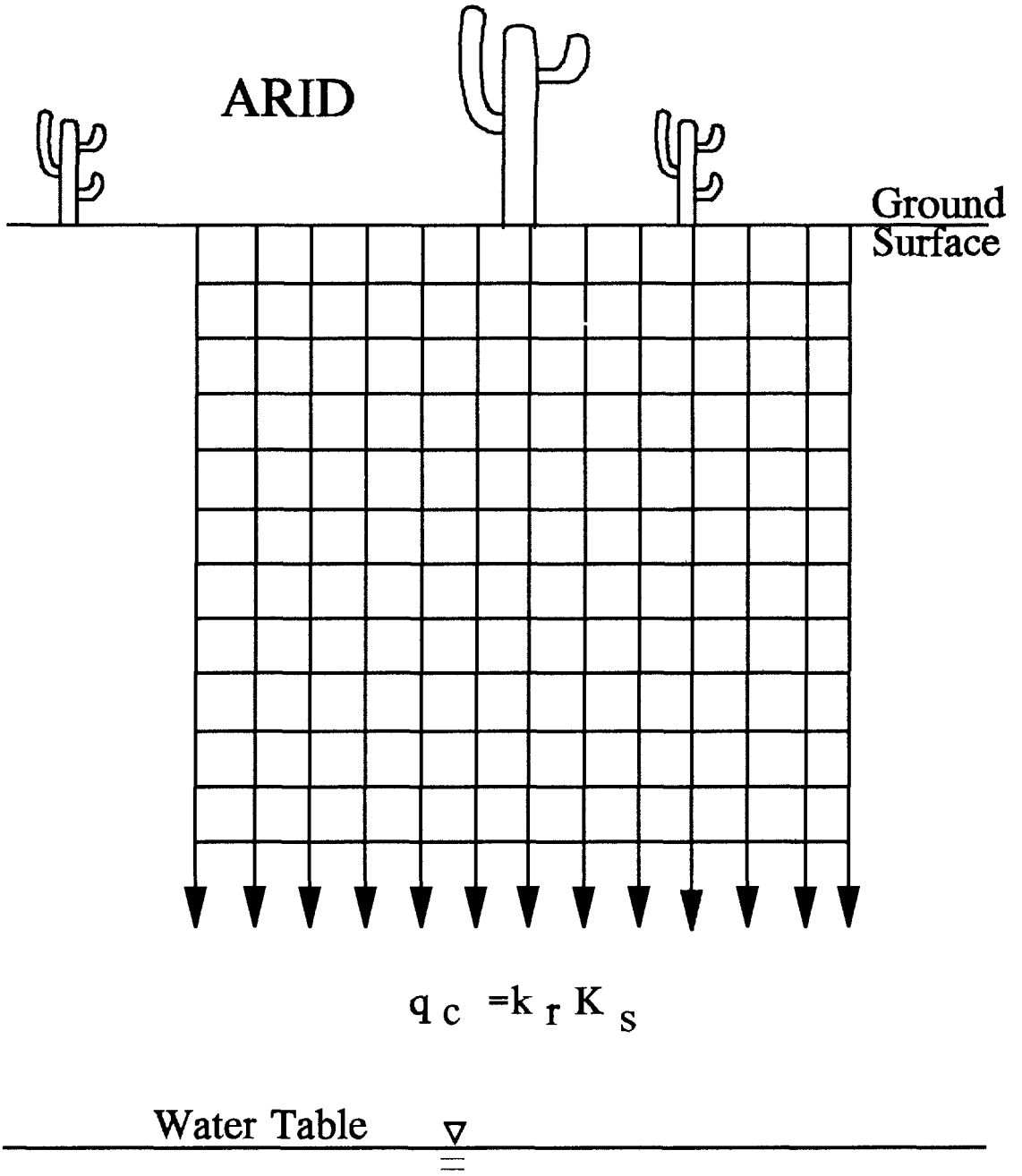


Figure 3.5 Use of a pressure-head gradient boundary condition to simulate a portion of the unsaturated zone.

$$h = h_p(x_b,y_b,z_b,t) \text{ on } B_v \quad (3\text{-}8a)$$

or

$$-n \cdot k_r K_s \cdot (\nabla h + \nabla z) = q_p(x_b,y_b,z_b,t) \text{ on } B_v \quad (3\text{-}8b)$$

and during periods of nonprecipitation are:

$$h = h_p(x_b,y_b,z_b,t) \text{ on } B_v \quad (3\text{-}8c)$$

or

$$h = h_m(x_b,y_b,z_b,t) \text{ on } B_v \quad (3\text{-}8d)$$

or

$$-n \cdot k_r K_s \cdot (\nabla h + \nabla z) = q_e(x_b,y_b,z_b,t) \text{ on } B_v \quad (3\text{-}8e)$$

where

h_p = maximum pressure head (L)
q_p = maximum infiltration rate (L/T)
h_m = minimum pressure head (L)
q_e = maximum evapotranspiration rate (L/T)
B_v = portion of the system boundary subject to a variable boundary condition

Physically, the maximum pressure head limit on the boundary prevents the generation of inappropriate surface water mounding. The minimum pressure head restraint keeps the evaporation process from drying the soil near the boundary to moisture levels lower than residual saturation levels. The variable boundary condition can be used to approximate seepage faces within the studied area.

Internal source/sink terms, as represented by the term q ($L^3/T/L^3$) in Equation 3-1 are also accounted for in 3DFEMWATER. As with the boundary conditions, the source/sink terms can be constant or allowed to vary with time. Two source/sink options are available in the code. The first is a distributed source/sink option and the second is a point source/sink option.

The distributed source option is a source intensity that is integrated over the volume of an element. The user prescribes a source intensity, q_2 ($L^3/T/L^3$), or flux rate per unit volume for each distributed source element. This option allows a user modeling a large area to approximate the influence of several wells within an element.

The point source/sink option is generally used to represent production or injection wells. Wells are represented as volumetric water fluxes, q_1 (L^3/T), applied at a nodal point or, to better represent a screening interval, a column of nodal points (Figure 3.6). If

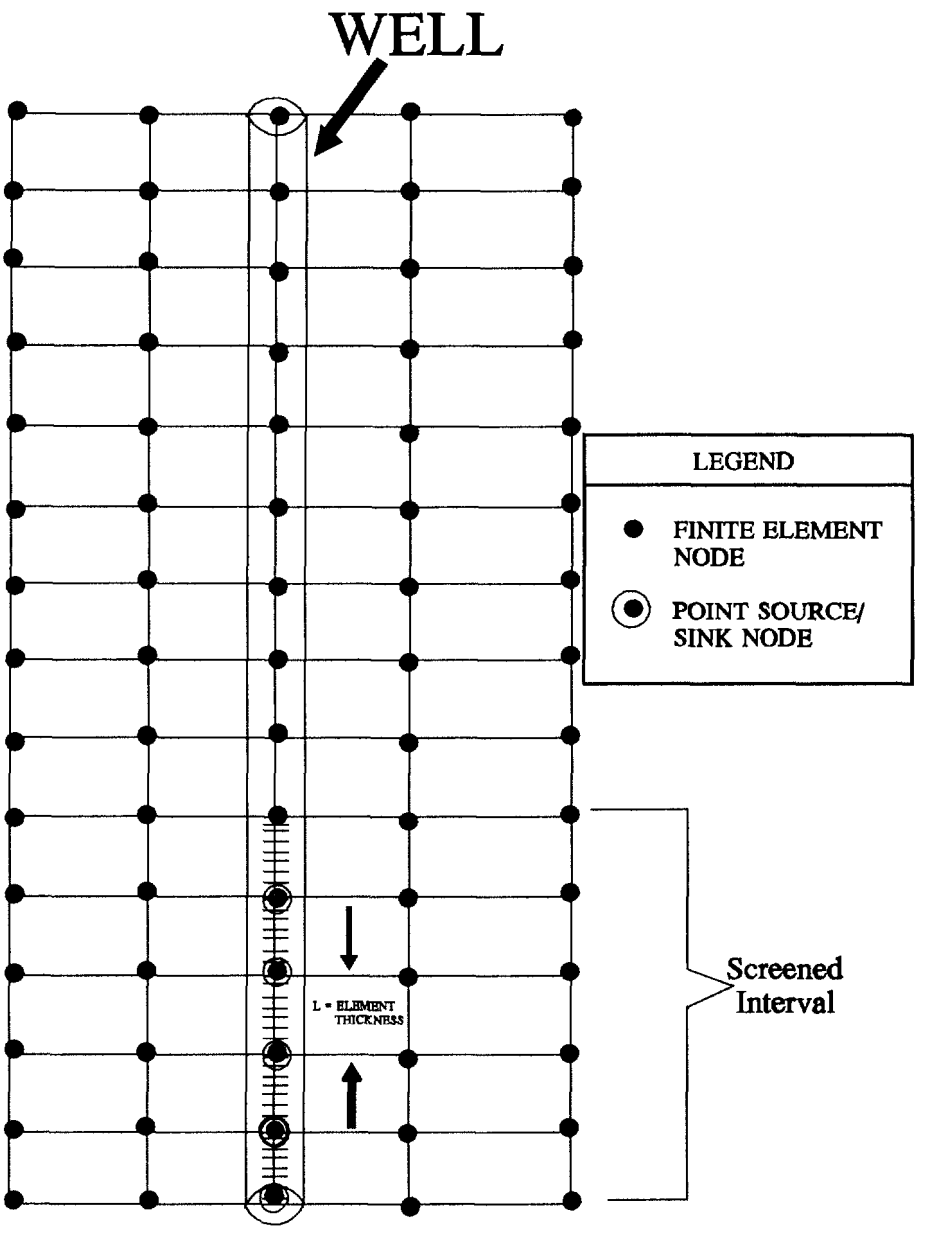


Figure 3.6. Using a series of nodes to represent a screened well interval.

vertically adjacent nodes are used to represent the screened interval of a well, the volumetric flux must be distributed among the nodes. The most appropriate distribution of the total flux is in proportion to the effective conductance, C_e, of the individual nodes where the effective conductance of each node is defined as:

$$C_e = 0.5\left[(K_s)_{n-1}L_{n-1} + (K_s)_n L_n\right] \tag{3-9}$$

where n-1 and n are indices referring to the element below the node and the element above the node, respectively, and 0.5L is half the thickness of an element.

Time-variant boundary conditions and source/sink flux or flux intensity rates are defined by a series of paired time and value points. This paired data is used to assemble a look-up table from which appropriate values are obtained using linear interpolation at specified times of analysis. Constant values can be specified by assigning the same value to a set of two time/data point pairs, making sure that the simulation time is fully spanned.

3.1.3 Initial Conditions

The solution of Richard's equation also requires the initialization of pressure head values such that:

$$h = h_i(x,y,z,t=0) \text{ in } R \tag{3-10}$$

where h_i is the initial pressure head distribution (L), and R is the region of interest (Figure 3.7). Besides providing a frame of reference for transient analyses, the initial conditions are used to set the nonlinear parameters at the beginning of a simulation. For transient problems, an appropriate set of initial pressure head values may either be input directly or derived from a steady-state simulation. For more information on these options see Section 4.1.11.

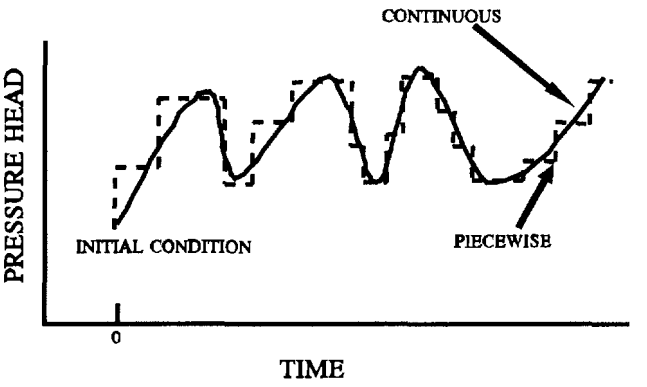


Figure 3.7. Pressure head versus time at a nodal point on the finite element grid.

3.1.4 Steady-State

When analyzing the influence of transient stresses, such as well production schemes and drought conditions, on the flow system, a starting point must be assumed. The user defines boundary conditions and flow parameters as best he/she can, then does an initial simulation to allow the system to reach an equilibrium or steady-state (Figure 3.8). The steady-state simulation then defines the pressure head at all points in the system and it is from this initial condition that a transient simulation is started. Although the actual system is never really in steady-state, by using averaged conditions (i.e., rainfall, etc.) a reasonable starting point is generated. If the steady-state simulation fails to converge or the results poorly match field data, flow parameters and/or boundary conditions should be adjusted to improve the starting conditions. The steady-state or equilibrium condition is generated by removing the temporal term from Equation 3-1. The system is then defined as the equilibrium reached under the average conditions.

Besides being used for initial conditions for a transient simulation, the steady-state flow option can also be used in conjunction with a transient transport simulation. Since the flow system will generally reach equilibrium under non-changing stresses faster than an associated solute transport problem, using a steady-state flow field and average conditions to define the advective portion of solute transport will often give a good approximation of the change of solute distribution over time. The savings in computational effort can be considerable and, given the uncertainty of parameters in the system, an acceptable approximation may be reached.

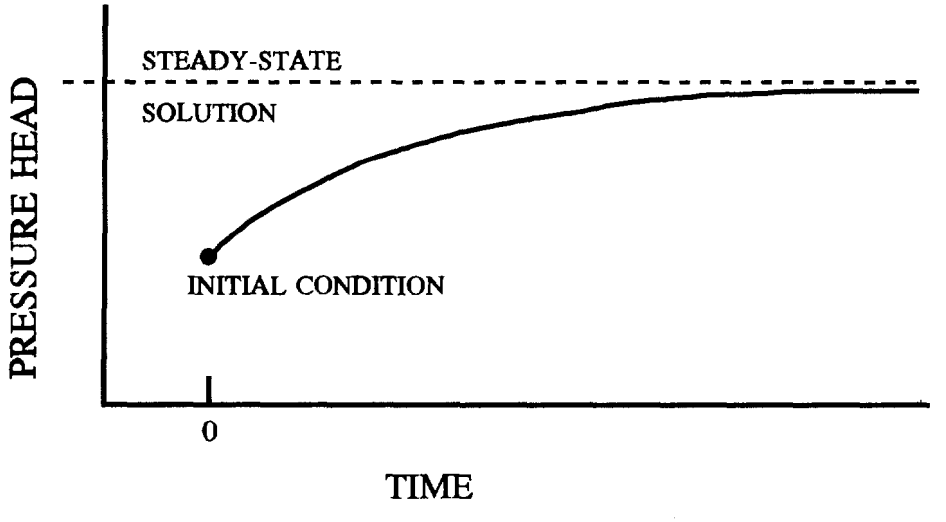


Figure 3.8 Pressure head versus time at a nodal point where a steady-state solution is being approached.

3.2 NUMERICAL APPROXIMATION IN 3DFEMWATER

The 3DFEMWATER model was developed to solve the variably-saturated flow equation described in Section 3.1. In the model, Richard's equation (Equation 3-1) is approximated using the Galerkin finite element technique. The time integral term in Equation 3-1 is approximated using backwards or central (Crank-Nicholson) difference in time. The nonlinearity of the system is treated using Picard iteration and the generated set of linearized equations is solved using a block iterative method.

3.2.1 Galerkin Formulation

In 3DFEMWATER, Richard's equation is approximated using the Galerkin finite element method (Pinder and Gray, 1977) where the dependent variable, pressure head, is approximated by a trial function of the form:

$$h = N_j(x_i,t)h_j(t) \quad j = 1,2,\ldots,n \tag{3-11}$$

where $N_j(x_i,t)$ are the three-dimensional shape functions and $h_j(t)$ are nodal values of pressure head at time t for the n nodes of which the finite element grid is comprised (Figure 3.9).

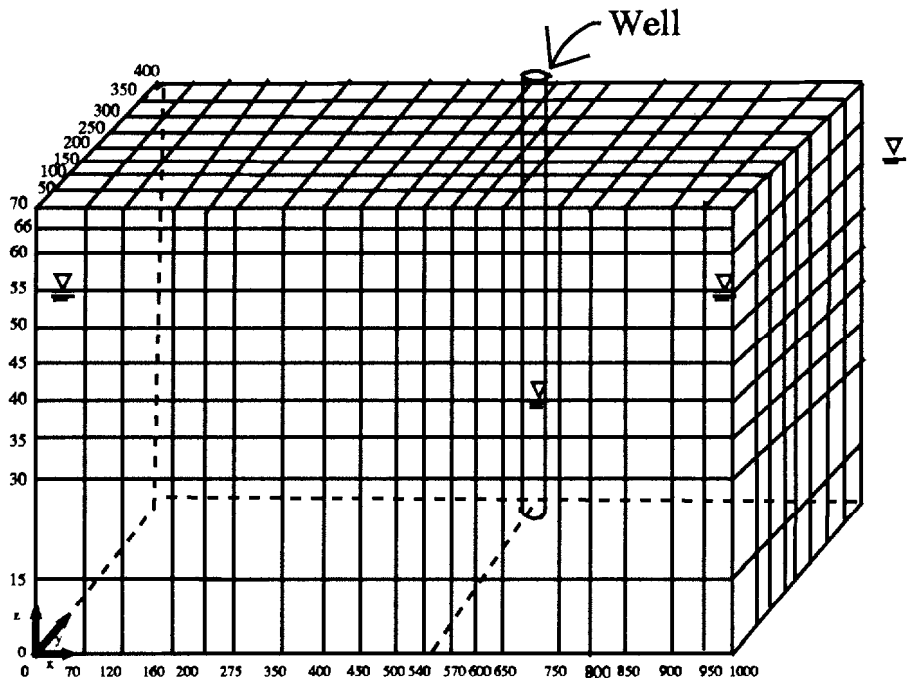


Figure 3.9. Finite element grid for production from a single well in a variably-saturated porous medium.

Substituting the trial functions into Equation 3-1 and applying the Galerkin criterion, we generate a set of weighted residual minimization equations:

$$\int_{R_s} W_i \left[F(h) \frac{\partial \hat{h}}{\partial t} - \nabla \cdot [k_r K_s (\nabla \hat{h} + \nabla z)] - q \right] dR = 0 \qquad (3\text{-}12)$$

where W_i are the weighting functions and R_s is the volume being simulated.

For the Galerkin method, the weighting functions are the same as the shape functions. Substituting $W_i = N_i$ and Equation 3-1 into Equation 3-12 results in:

$$\int_{R_s} N_i \left[F(h) \frac{\partial (N_j h_j)}{\partial t} - \nabla \left[k_r K_s (h_j \nabla N_j + \nabla z) \right] - q \right] dR = 0, \quad \begin{matrix} i = 1,2,...n \\ j = 1,2,...n \end{matrix} \qquad (3\text{-}13)$$

where n is the number of nodes. Integration by parts can be used to rid Equation 3-13 of all second order derivatives, leaving a set of equations of the form:

$$\begin{aligned} &\int_{R_s} F(h) N_i \frac{\partial (N_j h_j)}{\partial t} dR + \int_{R_s} k_r K_s \nabla N_i \cdot (h_j \nabla N_j + \nabla z) dR \\ &\quad - \int_{B_s} N_i \mathbf{n} \cdot k_r K_s (h_j \nabla N_j + \nabla z) dB - \int_{R_s} N_i q dR = 0 \end{aligned} \qquad (3\text{-}14)$$

where B_s is the region boundary. The integrals given in Equation 3-14, which are taken over the entire region being modeled, can be replaced by the summation of integrals taken over the individual elements of which the finite element grid (Figure 3.9) consists. This finite element approximation generates a set of n nodal equations of the form:

$$A_{ij} \frac{dh_j}{\partial t} + B_{ij} h_j = C_i, \quad \begin{matrix} i = 1,2,...n \\ j = 1,2,...n \end{matrix} \qquad (3\text{-}15a)$$

where

$$A_{ij} = \sum_{k=1}^{m} \int_{R_s} F(h) N_i^e N_j^e dR \qquad (3\text{-}15b)$$

$$B_{ij} = \sum_{k=1}^{m} \int_{R_e} \nabla N_i^e \cdot k_r K_s \cdot \nabla N_j^e dR \qquad (3\text{-}15C)$$

and

$$C_i = \sum_{k=1}^{m} -\left[\int_{R_e} k_r K_s \cdot \nabla N_i^e \cdot \nabla z dR + \int_{R_e} N_i^e q dR + \int_{B_e} N_i^e \mathbf{n} \cdot k_r K_s \cdot (h_j \nabla N_j^e + \nabla z) dB \right] \qquad (3\text{-}15d)$$

where m is the number of elements into which the system is discretized and N^e denotes elemental shape functions.

3.2.2 Solution Techniques

To solve the series of linearized ordinary differential equations presented in Equation 3-15a, the time differential is replaced by a finite difference formulation, resulting in working equations for 3DFEMWATER of the form:

$$\frac{A_{ij}}{\Delta t_k} \left(h_j^{k+1} - h_j^{k} \right) + w B_{ij}^{k+w} h_j^{k+1} + (1-w) B_{ij}^{k+w} h_j^{k} = C_i^{k+w} \qquad (3\text{-}16)$$

where k+l represents the current time level, k the previous time level, At the length of the current time step and w the time weighting function (1.0=backwards in time; 0.5= Crank Nicholson or centered in time). Note that the associated transport code, 3DLEWASTE, utilizes a backwards-in-time scheme: Therefore, when using 3DFEMWATER to generate a flow field for a 3DLEWASTE simulation, the backwards-in-time option should be used. This prevents the possibility of a mismatch in the interpolation of time-variant boundary condition and source/sink flux values.

For each time step, the solution method involves an outer and inner iterative scheme (Figure 3.10) where the outer iterations control convergence of the nonlinear terms in the equations and the inner iterative scheme controls the block-iterative method of solving the linearized set of equations. For each nonlinear iteration, the linearized set of equations is solved using relative permeability and storage terms updated using pressure head values generated during the previous nonlinear (outer) iteration. Relative permeability and storage terms for the first iteration in a time step are based on pressure head values from the previous time step, or for the first time step, from the initial conditions.

Because of the strong nonlinear nature of the soil moisture curves, the outer iterative scheme may become unstable. To help circumvent this problem it is often helpful to damp the iterative changes in the pressure head. One method of damping the iterative changes is through the use of an under-relaxation factor. Implementation of the under-relaxation factor for the outer iterations in 3DFEMWATER is as follows:

where u is the outer under-relaxation factor and r is the iteration number. If damping is needed, values below one should be used. Acceleration or over-relaxation ($1.0<u<2.0$)

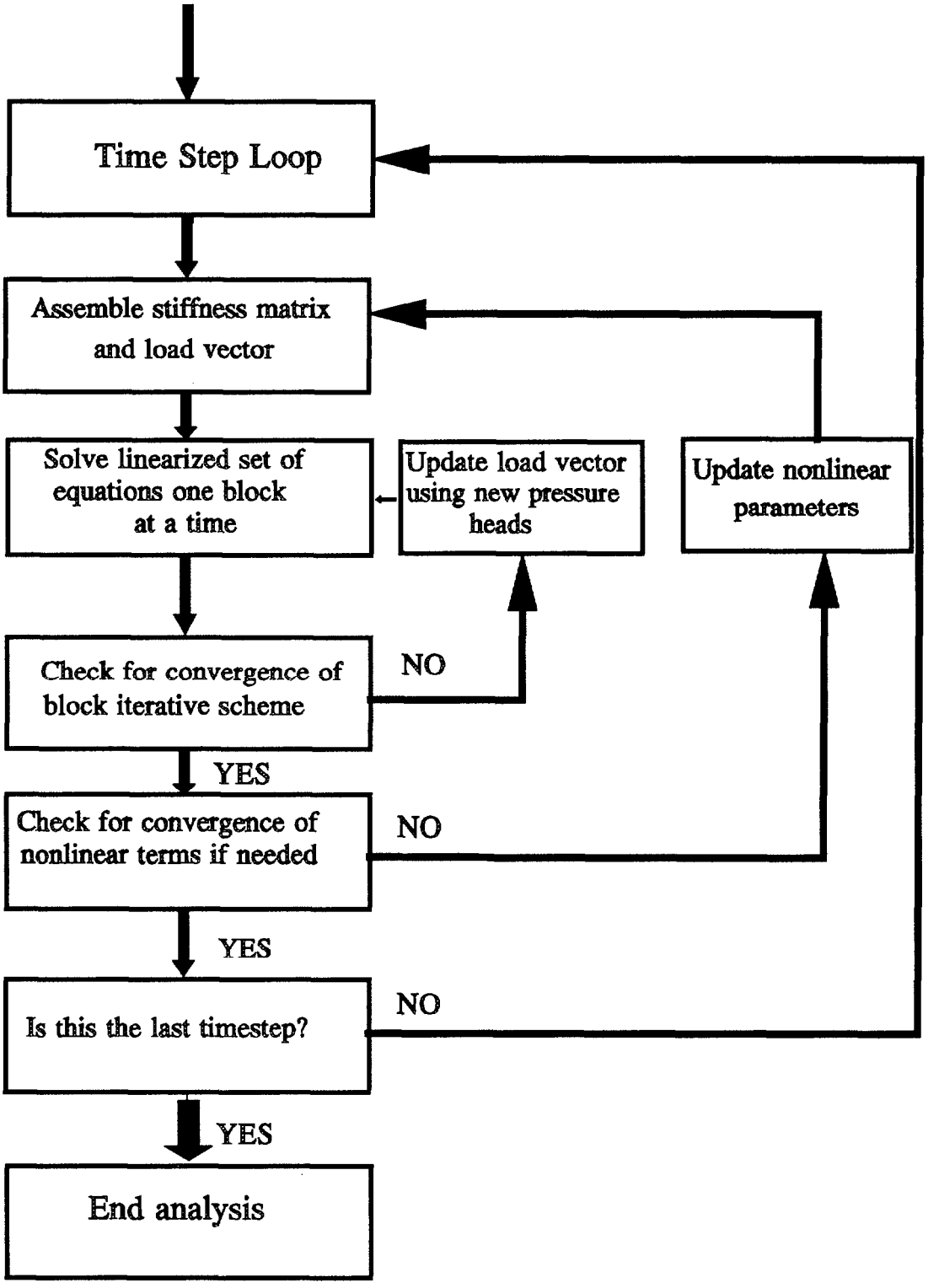


Figure 3.10. Solution scheme for unsaturated flow analysis.

$$h_i^{r+1} = (1 - u)h_i^r + uh_i^{r+1} \quad (3\text{-}17)$$

is generally not recommended for the nonlinear iterations as it may make the solution become unstable. For transient simulations, reduction of the time-step size can also help increase the stability of the solution scheme. Note that sometimes steady-state problems will be difficult to solve. In this case, it is often worth trying a transient solution approach, using expanding time steps to approach the steady-state solution.

For each nonlinear iteration, a set of linearized simultaneous equations is solved using a block iterative scheme. The user defines a set of subregions (or blocks) by prescribing the nodes contained in each subregion (Figure 3.11). The code then generates a series of connectivity arrays indicating: 1) the nodes contained in each subregion, 2) for each node, all other nodes found in elements it is part of, and 3) which of these adjacent nodes are located in the same subregion. The nodal equations for each subregion are solved directly using a Gaussian solver. For each nodal equation defined in Equation 3-15a, contributions from adjacent nodes falling outside the subregion being solved for are generated by multiplying the matrix terms with the appropriate nodal pressure heads. These pressure heads are generated during the last direct solution for the subregion containing the adjacent nodes.

Subregions are generally defined as nodal planes (Figure 3.11) allowing the user to work with a minimal half-bandwidth when the direct solver is invoked. The half-bandwidth is defined as one plus the largest difference between the node number associated with the nodal equation and the other nodes found in elements the node is part of and which are in the same block as the node. As a general rule, subregions comprised of vertical or sub-vertical nodal slices provide the smallest half-bandwidth and will perform well in the block iterative method, although this may not always be the case. For some problems, horizontal slicing may be advantageous. The block iterative logic contains a relaxation factor which can be used to over-relax the solution and help accelerate the rate of convergence. Implementation of the inner over-relaxation scheme is as follows:

$$h_i^{s+1} = (1 - o)h_i^s + oh_i^{s+1} \quad (3\text{-}18)$$

where s denotes the inner iteration number and o is the over-relaxation factor. The optimal value of the over-relaxation factor usually falls between 1.5 and 1.9. A good starting point is o = 1.72.

3.3 3DLEWASTE

3DLEWASTE is designed to simulate the movement of dissolved species through a variably-saturated porous medium. Typical applications for 3DLEWASTE include the examination of: 1) leachate migration from landfills and surface impoundments, 2) the influence on water quality of pesticide and fertilizer applications, and 3) the environmental impact of leaky containment structures such as underground and above ground storage tanks (Figure 3.12). Velocity fields needed to define the advective pathways of water bearing the chemicals are provided by associated 3DFEMWATER simulations.

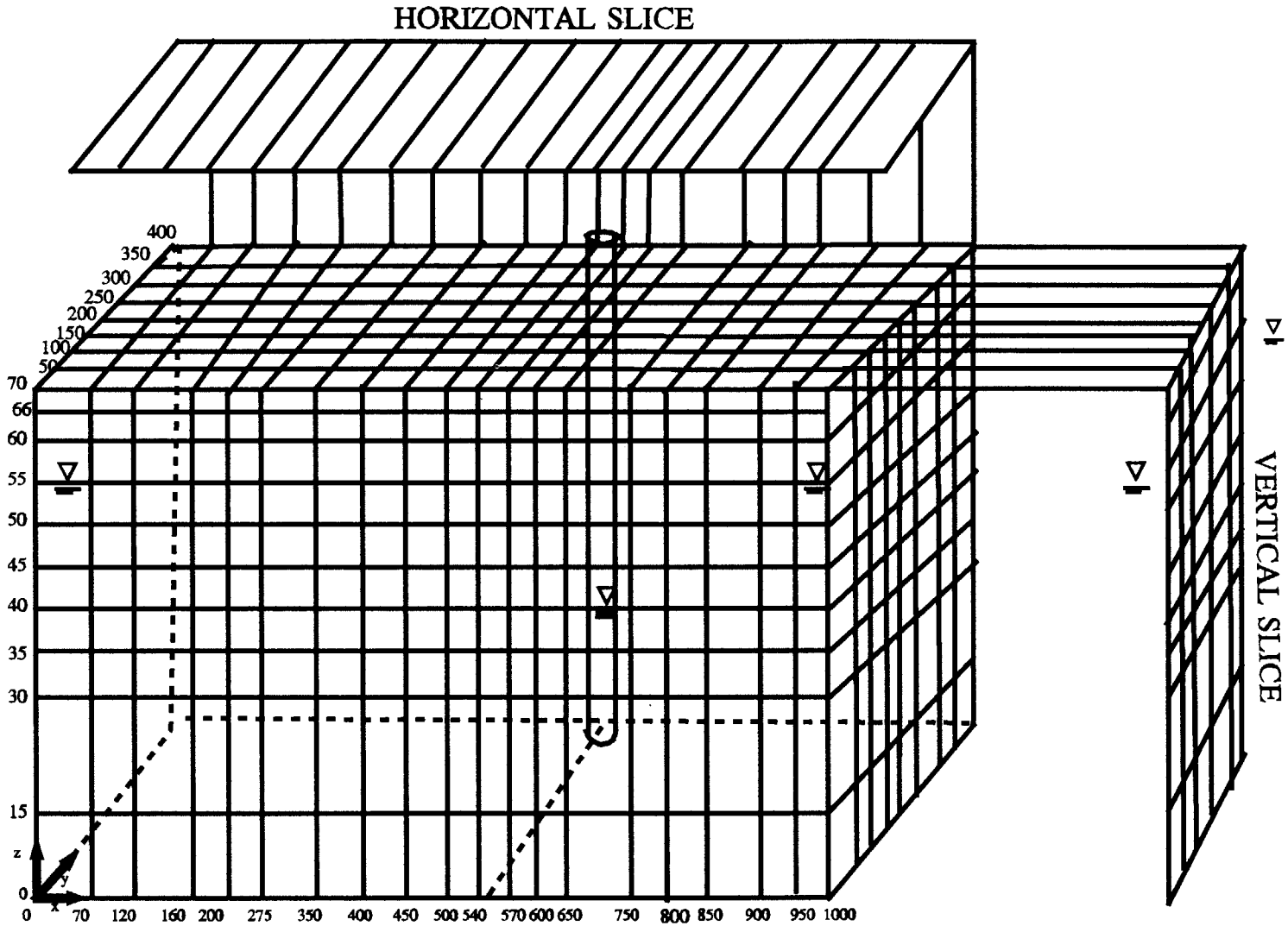


Figure 3.11. Use of vertical or horizontal nodal slices in the block interative method.

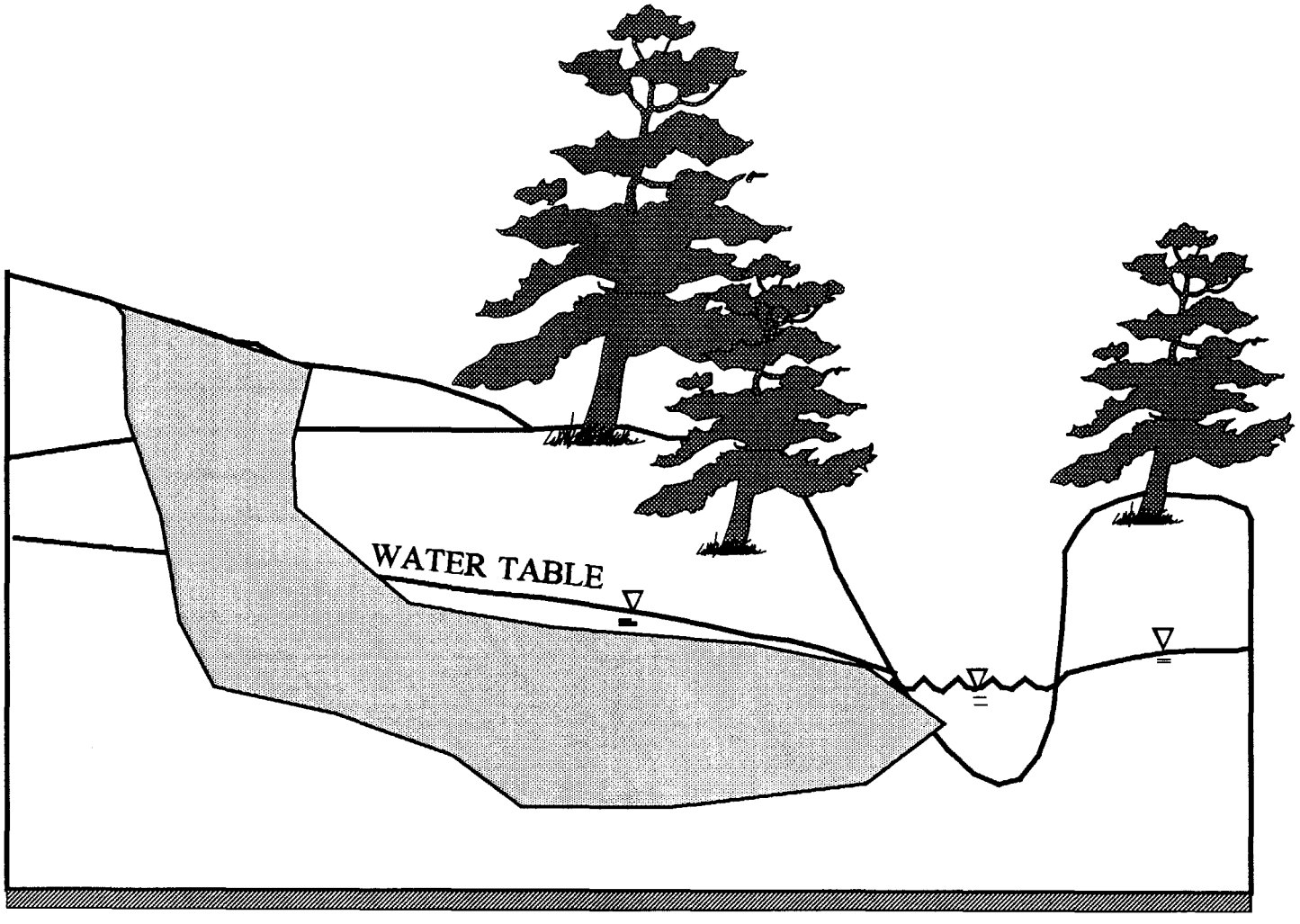


Figure 3.12. Migration of dissolved contaminants through the unsaturated zone into an unconfined aquifer system.

3.3.1 Governing Equations

The governing equation for advective-dispersive solute transport through variably-saturated porous media, based on the laws of conservation of mass and flux, can be written in the form:

$$\theta\frac{\partial C}{\partial t} + \rho_b\frac{\partial S}{\partial t} = \nabla\cdot(\theta\mathbf{D}\cdot\nabla C) - \mathbf{V}\cdot\nabla C - \lambda(\theta C + \rho_b S) + QC_{in} - QC \qquad (3\text{-}19)$$

where

θ = moisture content (L^3/L^3)
ρ_b = bulk density of the porous medium (M/L^3)
C = concentration of the dissolved species (M/L^3)
S = species concentration in the adsorbed phase (M/M)
t = time (T)
$\mathbf{V}$ = Darcy velocity (i.e., specific discharge) (L/T)
$\nabla\cdot$ = del operator indicating divergence
∇ = del operator indicating gradient
$\mathbf{D}$ = dispersion coefficient tensor (L^2/T)
λ = material decay constant (T)
Q = water source/sink rate (M/T)
C_{in} = dissolved species concentration of the source/sink fluid (M/L^3)

Note that for a fluid sink, such as a production well, $C_{in} = C$.

The dispersion coefficient tensor, **D,** which defines the spreading of the dissolved species as it is advected through the system, is defined as:

$$\theta\mathbf{D} = \alpha_T|\mathbf{V}|\delta + (\alpha_L - \alpha_T)\mathbf{VV}/|\mathbf{V}| + \theta a_m\tau\delta \qquad (3\text{-}20)$$

where

$|V|$ = magnitude of the Darcy velocity vector (L/T)
δ = Kronecker delta tensor
α_L = longitudinal dispersivity (L)
α_T = transverse dispersivity (L)
a_m = molecular diffusion coefficient (L^2/T)
τ = tortuosity coefficient (--)

The dispersivity parameters quantify the magnitude of longitudinal and lateral spreading of the dissolved species as it is advected through the system. This spreading, called hydrodynamic dispersion, is due to the combined influence of 1) water movement through the complex pathways, and 2) associated mixing patterns (Figure 3.13) that occur over spatial scales not accounted for by the flow field approximated in the advective term of Equation 3-19. These complex pathways may vary in scale from pore spaces and microfractures to larger scale features such as joints and fracture zones. Since dispersion is a function of features of various scales, the appropriate value of dispersivity must take into consideration the distance the species travels. The

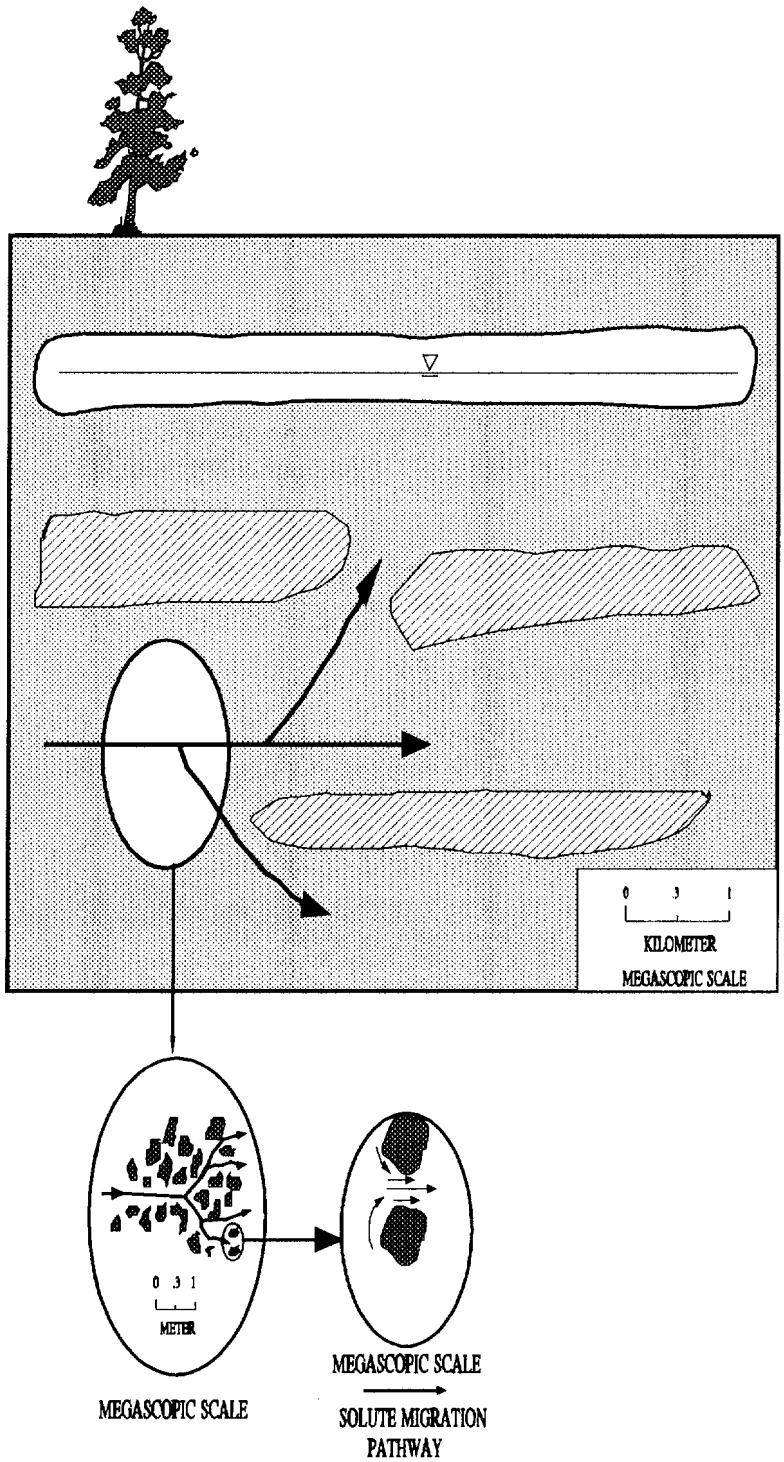


Figure 3.13. Diagram showing the effect of scale on hydrodynamic dispersion processes.

molecular diffusion coefficient in Equation 3-20 quantifies the spreading due to molecular diffusion.

In order to solve Equation 3-19 for a single dependent variable, the constitutive relationship between the species concentrations in the dissolved and adsorbed phases must be defined. The 3DLEWASTE code allows the user to choose from three relationships: 1) alinear isotherm, 2) Freundlich isotherm, or 3) Langmuir isotherm. The isotherms, as determined in laboratory partitioning experiments, can be plotted in log-log form to derive:

$$\log S = n \log C + \log K \tag{3-21}$$

or

$$S = KC^{n} \tag{3-22}$$

where n is slope of the plot of log S versus log C and K is the S-axis intercept (Freeze and Cherry, 1979). Equation 3-22 defines the Freundlich isotherm, which is often used to describe the partitioning between the dissolved and absorbed phases. When the isotherm has a slope n= 1, the isotherm is linear and the relationship can be defined as:

$$\frac{dS}{dC} = K_d \tag{3-23}$$

where K_d is called the distribution coefficient (L^3/M). Linear isotherms are often used to describe the adsorption of hydrophobic organic compounds to organic matter in soils. The distribution coefficient is described as a function of the organic carbon content of the soil as:

$$K_d = f_{oc} K_{oc} \tag{3-24}$$

where f_{oc} is the fractional organic carbon content and K_{oc} is the normalized distribution coefficient. There are many published lists of values for K_{oc} (e.g., Lyman et al., 1982; U.S. EPA, 1986; Verschueren, 1983). Data are available primarily for pesticides and, to a lesser degree, aromatic and polycyclic aromatic compounds. If data on K_{oc} are not available for a particular chemical, a value can be estimated from empirical relationships between K_{oc} and some other property of the chemical such as the water volubility, S, the octanol-water partition coefficient, K_{ow}, or the bioconcentration factor for aquatic life, BCF. Lyman et al. (1982) tabulate 12 such regression equations obtained from data sets of different classes of chemicals. One commonly-used relationship (Karickhoff et al., 1979) takes the form:

$$K_{oc} = 0.41 K_{ow} \tag{3-25}$$

The Langmuir isotherm takes the form:

$$S = \frac{S_{max} KC}{1 + KC} \tag{3-26}$$

where S_{max} is the maximum concentration allowed in the medium.

The effective decay constant, λ, is a degradation constant that can be used to quantify the effects of radioactive decay, or the composite effects of hydrolysis and biodegradation. When used to quantify the effects of hydrolysis and biodegradation, the effective decay coefficient (for a linear isotherm) takes the form:

$$\lambda = \frac{\lambda_1 \theta + \lambda_2 K_d \rho_b}{\theta + K_d \rho_b} + \lambda_b \tag{3-27}$$

where λ_1 is the first-order hydrolysis rate constant for the dissolved species, λ_2 is the first-order hydrolysis rate constant for the sorbed species, and λ_b is the first-order biodegradation rate constant. The dissolved species first-order hydrolysis rate can be written in terms of the acid-catalyzed (K_a), base-catalyzed (K_b), and neutral (K_n) hydrolysis rate constants as:

$$\lambda_1 = K_a[H = K_a[H^+] + K_n + K_b[OH^-] \tag{3-28}$$

where [H+] is the hydrogen ion concentration and [OH-] is the hydroxyl ion concentration. The sorbed phase first-order hydrolysis rate is considered to be a function of the acid and neutral hydrolysis rates and is usually written in the form:

$$\lambda_2 = \alpha K_a[H^+] + K_n \tag{3-29}$$

where α is the acid-catalyst hydrolysis rate enhancement factor for the sorbed phase with a typical value of 10.0. Note that for a nonlinear isotherm the formulation in 3DLEWASTE is valid only if $\lambda_1 = \lambda_2$.

The governing equation for advective-dispersive solute transport in a porous medium, as presented in Equation 3-19, describes the transport from an Eulerian or fixed framework. The numerical algorithm may begin to oscillate and fail to converge to a solution of this equation when the advective term starts to dominate over the dispersive term and the equation takes on a hyperbolic nature. Dominance of the advective term over the dispersive term is reflected in the non-dimensional Peclet number, which is defined as the ratio of the product of the velocity magnitude and distance advected to the dispersion coefficient. In finite element analysis the critical Peclet number is the local Peclet number of an element, where the local Peclet number is defined as:

$$P = L/\alpha_L \tag{3-30}$$

where L is the element length.

One method of circumventing the numerical problems (i.e., oscillation and failure to converge) associated with Peclet numbers greater than 2 is to address the system through a moving (i.e., Lagrangian) coordinate system. In the Lagrangian formulation

for solute transport in a porous medium, the temporal term is defined as a material derivative of the form:

$$\left(\theta + \rho_b \frac{dS}{dC}\right)\frac{DC}{Dt} = \theta \frac{\partial C}{\partial t} + \rho_b \frac{\partial S}{\partial t} + \mathbf{V}\cdot\nabla C \tag{3-31}$$

where D denotes the material derivative.

The advective term, $\mathbf{V}\cdot\nabla C$, written in index notation becomes:

$$\mathbf{V}\cdot\nabla C = \frac{dx_i}{dt}\frac{\partial C}{\partial x_i} \tag{3-32}$$

where the repeated indices indicate summation. Substituting Equation 3-31 into Equation 3-19, the governing equation for a Lagrangian framework becomes:

$$\left(\theta + \rho_b \frac{dS}{dC}\right)\frac{DC}{Dt} = \nabla\cdot(\theta\mathbf{D}\cdot\nabla C) - \lambda(\theta C + \rho_b S) + QC_{in} - QC \tag{3-33a}$$

for a linear isotherm. The average linear velocity, $\mathbf{V}^*$, for a linear isotherm becomes:

$$\mathbf{V}^* = \mathbf{V}/\left(\theta + \rho_b \frac{dS}{dC}\right) \tag{3-33b}$$

For a non-linear isotherm, the Lagrangian equation becomes:

$$\theta\frac{DC}{Dt} + \rho_b\frac{dS}{dC}\frac{\partial C}{\partial t} = \nabla\cdot(\theta\mathbf{D}\cdot\nabla C) - \lambda(\theta C + \rho_b S) + QC_{in} - QC \tag{3-34a}$$

where

$$V^* = \mathbf{V}/\theta \tag{3-34b}$$

Full implementation of the Lagrangian approach implies the solution of Equation 3-33 using a moving coordinate system. Another method of circumventing the instability problem is to utilize a hybrid Eulerian-Lagrangian approach. Such an approach is implemented in 3DLEWASTE. In the hybrid approach, the advective term of the material derivative is evaluated in a Lagrangian manner by a backwards particle tracking scheme (Figure 3.14). The particle tracking scheme generates a particle starting location and an associated concentration, C*. This concentration, C*, is the starting concentration of each particle which reaches a nodal point at the end of that particular time step. The material term of Equation 3-33 is then approximated by:

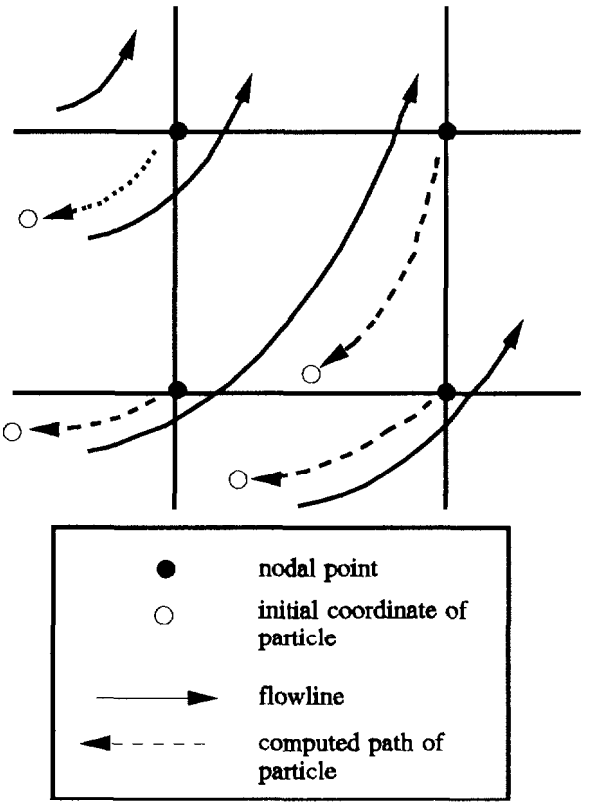


Figure 3.14. Backward particle tracking to determine the starting point of an advected particle.

$$\frac{DC}{Dt} = \frac{C - C^*}{\Delta t} \tag{3-35}$$

The diffusion-type equation is then solved using a fixed coordinate system. Note that for a steady-state simulation, where $\Delta t \rightarrow \infty$, the logic is implemented by multiplying the transient storage terms by zero and evaluating the advection term in a fixed coordinate system.

3.3.2 Boundary Conditions and Transient Source/Sink Terms

Unique solutions to advective-dispersive solute transport problems are generated by solving the governing equation (Equation 3-19) in conjunction with 1) a set of boundary conditions, defined at the physical edges of the modeled system, and where appropriate, 2) source/sink terms applied within the system (see Figure 3.4).

Boundary conditions and source/sink terms available in the 3DLEWASTE model include:

- Prescribed-concentration (Dirichlet) boundaries
- Specified-flux (Cauchy) boundaries
- Specified-dispersive-flux (Neumann) boundaries
- Variable boundaries
- Point sources
- Distributed sources

Prescribed-concentration or *Dirichlet* boundaries are defined by prescribing dissolved species concentrations at specified boundary nodes as:

$$C = C_d\,(x_b, y_b, z_b, t) \quad \text{on } B_d \tag{3-36}$$

where C_d is the specified solute concentration, B_d is the portion of the system boundary subject to a Dirichlet boundary condition, and (x_b, y_b, z_b) is the spatial coordinate on the boundary. Dirichlet boundaries are typically used to test computer programs by allowing comparisons with analytical solutions. Unlike the analogous constant-head boundaries of flow models, constant-concentration boundaries are generally poor approximations of contaminant source terms. Bodies of fresh water located upgradient from contaminant sources can be approximated using constant concentration nodes. When used to define sources, specified concentrations may be constant or allowed to vary with time, reflecting physical processes such as degradation of the source due to radioactive decay, hydrolysis, biodegradation, or physical removal. Concentration versus time profiles can be defined to account for seasonal or other time-variant changes in dissolved species levels.

The *specified-flux (Cauchy)* boundary represents the portions of the system boundary where infiltration can be quantified. The specified-flux boundary has many representations including: 1) infiltration due to leachate migration from a landfill or surface impoundment, 2) application of pesticides or fertilizer to fields, and 3) the dilution effects of rainfall or irrigation on previously applied constituents. The specified-flux boundary condition can be written:

$$n \cdot (VC - \theta D \cdot \nabla C) = q_c\,(x_b, y_b, z_b, t) \quad \text{on } B_c \tag{3-37}$$

where n is an outward unit vector normal to the boundary, $\theta D \cdot \nabla C$ is the dispersive flux caused by the concentration gradient VC, VC is the advective flux, q_c is the specified flux rate ($M/T/L^2$), and B_c is the portion of the system boundary subject to a specified-flux boundary condition. The specified boundary is simulated by assigning mass flux rates along specified element sides. Flux rate versus time profiles can be defined to account for seasonal or other time-variant changes in flux rates.

In addition to the user-supplied mass flux rates, 3DLEWASTE automatically accounts for the influence of the water entering the system along the boundary. The infiltration

of fresh water is simulated by applying the specified-flux boundary condition and setting the mass flux rate to zero. The automatically generated term accounting for water flow normal to the boundary will simulate the dilution due to infiltration.

Also available in 3DLEWASTE is a ***specified-dispersive-flux*** or ***Neumann*** boundary condition of the form:

$$\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C) = q_n(x_b, y_b, z_b, t) \text{ on } B_n \tag{3-38}$$

where q_n ($M/T/L^2$) is the portion of the boundary flux attributable to the concentration and B_n is the portion of the system boundary subject to a specified-dispersive-flux boundary condition. Note that exit boundaries can be declared using this boundary condition and letting $q_n=0$. This physically simulates mass being advected out of the system.

For solute transport, the ***variable composite*** boundary condition represents a combined specified-flux/dispersive-flux boundary which allows for time-variant itilltratiorJwater-loss rates. The boundary condition during infiltration is:

$$\mathbf{n}\cdot(\mathbf{V}C - \theta\mathbf{D}\cdot\nabla C) = \mathbf{n}\cdot\mathbf{V}C_v \ (x_b, y_b, z_b, t) \text{ on } B_v \text{ if } \mathbf{n}\cdot\mathbf{V}\leq 0 \tag{3-39a}$$

where $\mathbf{n}\cdot\mathbf{V}$ is the Darcy velocity or discharge normal to the boundary, C, is the concentration of the dissolved species in the water entering at the boundary, and B_v is the portion of the boundary subject to a variable boundary condition. When water is exiting at the boundary, the boundary condition defaults to the dispersive flux condition:

$$\mathbf{n}\cdot(-\theta\mathbf{D}\cdot\nabla C) = 0 \text{ on } B_v \text{ if } \mathbf{n}\cdot\mathbf{V} > 0 \tag{3-39b}$$

and mass is advected out of the system. Like the specified-flux boundary condition, the variable boundary can represent: 1) infiltration due to leachate migration from a landfill or surface impoundment, 2) application of pesticides or fertilizer to fields, and 3) the dilution effects of rainfall or irrigation on previously applied constituents. When the boundary being modeled may be either an exit or an infiltration boundary, such as a precipitation/ evapotranspiration boundary or a seepage face, the variable boundary condition is the proper choice. The variable boundary condition can also be used in a manner similar to the dispersive-flux condition to simulate strictly exit nodes.

Internal source/sink terms, as represented by the term QC_{in} in Equation 3-19 are also accounted for in 3DLEWASTE. As with the boundary conditions, the source/sink terms can be constant or allowed to vary with time. Both the fluid flux rate, Q, and the injected fluid species concentration, C_{in}, are allowed to vary with time. Two source/sink options are available in the code. The first is a point source/sink option and the second, a distributed source/sink option. The first option is generally used to represent production or injection wells. The fluid fluxes in wells are represented as volumetric water fluxes, q_1 (L^3/T), applied at a nodal point or to better represent a screened interval, a column of nodal points (see Figure 3.6). If vertically adjacent nodes are used to represent the screened interval of a well, the volumetric flux must be distributed

among the nodes. The most appropriate method of doing this is discussed in Section 3.1.2. Note that the applied fluid fluxes must match those used in the associated flow simulation.

The distributed source option is a source intensity that is integrated over the volume of an element. For a distributed source element, the user defines a fluid source intensity, q_2 ($L^3/T/L^3$), or fluid flux rate per unit volume for each distributed source element. This option allows a user modelling a large area to approximate the influence of a well field within an element.

Time-variant boundary conditions and source/sink flux or flux intensity rates are defined by a series of paired time and value points. The paired data are used to assemble a look-up table from which appropriate values are obtained using linear interpolation at specified times of analysis. Constant values can be specified by assigning the same value to a set of two time/data point pairs, making sure that the simulation time is fully spanned.

3.3.3 Initial Conditions

The solution of the governing equation for solute transport in a porous medium also requires the initialization of concentration values such that:

$$C = C_i(x,y,z,t= 0) \text{ in } R \tag{3-40}$$

where C_i is the initial concentration distribution and R is the region of interest. The initial conditions are used to define the starting water quality and soil concentration levels for determining the fate of the dissolved constituents. Besides providing a frame of reference for transient analyses, the initial conditions are used to set the storage parameters for Freundlich and Langmuir isotherms at the beginning of nonlinear simulations. For transient problems, an appropriate set of initial concentration values may either be input directly or derived from a steady-state simulation. For more information on these options see Section 4.2.10.

3.3.4 Steady-State

When looking for a bounding solution to determine the maximum possible concentration levels that may be reached in a solute transport problem, a steady-state option may be employed. In the steady-state case, the time derivatives in Equation 3-19 are discarded and the equation, including the advective term, is solved in an Eulerian or fixed-coordinate framework. Note that any solute source prescribed as a boundary condition or source term becomes modeled as an infinite source. For many systems this upper bound may be highly conservative. The steady-state option is of no use if the source is solely defined by initial conditions.

3.4 NUMERICAL APPROXIMATION IN 3DLEWASTE

The 3DLEWASTE model was developed to simulate advective-dispersive solute transport in variably-saturated porous media. In the model, the hybrid Eulerian-Lagrangian governing equation (Equation 3-33) is approximated using the Galerkin

finite element technique. The time integral term in Equation 3-33 is approximated using backwards differencing in time. The nonlinearity of the system is treated using Picard iteration and the generated set of linearized equations is solved using a block iterative method.

3.4.1 Galerkin Formulation

In 3DLEWASTE, the diffusion equation is approximated using the Galerkin finite element method where the dependent variable, concentration, is approximated by a trial function of the form:

$$C = N_j(x_i,t)C_j(t) \quad j = 1,2,...,n \tag{3-41}$$

where $N_j(x_i,t)$ are the three-dimensional shape functions and $C_j(t)$ are nodal values of concentration at time t for the n nodes of which the finite element grid is comprised (see Figure 3.9). Substituting the trial functions into Equation 3-33 and applying the Galerkin criterion, we generate a set of weighted residual minimization equations of the form:

$$\int_{R_e} W_i\left[(\theta+\rho_b K_d)\frac{DC}{Dt} - \nabla\cdot(\theta\mathbf{D}\cdot\nabla C) - \lambda(\theta+\rho_b K_d)C + QC_{in} - QC\right] dR = 0 \tag{3-42}$$

for the linear isotherm case, where W_i are the weighting functions. For the Galerkin method, the weighting functions are the same as the shape functions and, therefore, Equation 3-42 can be written in the form:

$$\int_{R_e} N_i\left[(\theta+\rho_b K_d)\frac{DC}{Dt} - \nabla\cdot(\theta\mathbf{D}\cdot\nabla C) - \lambda(\theta+\rho_b K_d)C + QC_{in} - QC\right] dR = 0 \tag{3-43}$$

Integration by parts can be applied to the dispersive term to eliminate all second order terms in Equation 3-43, leaving an equation of the form:

$$\begin{aligned}&\int_{R_e} N_i(\theta+\rho_b K_d)N_j\frac{dC_j}{Dt}dR + \int_{R_e}\nabla N_i\cdot\theta\mathbf{D}\cdot\nabla N_j dRC_j - \int_{B_e}\mathbf{n}\cdot\theta\mathbf{D}\cdot\nabla N_j dBC_j \\ &+\int_{R_e}\lambda(\theta+\rho_b K_d)N_i N_j dRC_j - \int_{R_e}\frac{\partial\theta}{\partial t}N_i N_j dRC_j - \int_{R_e} QC_{in}N_i dR + \int_{R_e} QN_i N_j dRC_j = 0\end{aligned} \tag{3-44}$$

where B_e is the entire region boundary. The integrals given in Equation 3-44, which are taken over the entire region being modeled, can be replaced by the summation of integrals taken over the volumes and surfaces of individual elements of the finite element grid. This finite element approximation generates a set of n nodal equations of the form:

$$A_{ij}\frac{dC_j}{dt} + (B_{ij} + E_{ij})C_j = R_{ij} \qquad \begin{matrix} i = 1,2,...n \\ j = 1,2,...n \end{matrix} \tag{3-45a}$$

where

$$A_{ij} = \sum_{k=1}^{m} \int_{R_e} (\theta + \rho_b K_d) N_i^e N_j^e dR \tag{3-45b}$$

$$B_{ij} = \sum_{k=1}^{m} \int_{R_e} \nabla N_i^e \cdot \theta \mathbf{D} \cdot \nabla N_i^e dR \tag{3-45c}$$

$$E_{ij} = \sum_{k=1}^{m} \int_{R_e} N_i^e \left[\lambda(\theta + \rho_b K_d) + Q\right] N_j^e dR \tag{3-45d}$$

and

$$R_{ij} = \sum_{k=1}^{m} \left[\int_{R_e} Q C_{in} N_i^e dR + \int_{B_e} n \cdot \theta \mathbf{D} C_j \nabla N_j^e dB \right] \tag{3-45e}$$

where m is the number of elements into which the system is discretized and N^e are the elemental shape functions. Note that for a steady-state simulation, the full Eulerian approach is used. The Lagrangian term DC/Dt is replaced by $\partial C/\partial t$ and the Eulerian term:

$$\sum_{k=1}^{M} \int_{R_e} N_i^e \mathbf{V} \cdot \nabla N_j^e dR \tag{3-46}$$

is added to B_{ij}.

3.4.2 Solution Techniques

To solve the series of linearized ordinary differential equations represented by Equation 3-45a, the time differential is replaced by a finite difference formulation, resulting in working equations for 3DLEWASTE of the form:

$$\frac{A_{ij}}{\Delta t}\left(C_j^{k+1} - C_j^{*k}\right) + \left(B_{ij}^{k+1} + E_{ij}^{k+1}\right) C_j^{k+1} = R_i^{k+1} \qquad (3\text{-}47)$$

where k+1 represents the current time step, k the previous time step, and At the length of the current time step. Note that since the transient solution scheme allows only for a backwards difference approximation the associated flow runs should also be solved using backwards-in-time approximation.

For each time step, the solution method involves an inner iterative scheme (see Figure 3.10) which controls the block iterative method of solving the linear equations. For simulations where the nonlinear Freundlich or Langmuir isotherms are used, the solution method also involves an outer iterative scheme where the iterations control convergence of the nonlinear terms in the linearized set of equations. For each nonlinear iteration, the linearized set of equations is solved using storage terms updated using concentration values from the previous nonlinear (outer) iteration. Storage terms for the first iteration in a time step are based on concentration values from the previous time step, or for the first time step, from the initial conditions. If the outer iterative scheme becomes unstable, it may be helpful to damp the iterative changes in the concentration. One method of damping the iterative changes is through the use of an under-relaxation factor. Implementation of the under-relaxation factor for the outer iterations in 3DLEWASTE is:

$$C_i^{r+1} = (1 - u_o) C_i^r + u_o C_i^{r+1} \qquad (3\text{-}48)$$

where u_o is the outer under-relaxation factor and r is the iteration number. If damping is needed, values between 0.5 and 0.9 should suffice. Acceleration or over-relaxation ($1.0<u_o<2.0$) is generally not recommended for the nonlinear iterations as it may make the solution become unstable.

The linear or linearized set of simultaneous equations is solved using a block iterative scheme. The user defines a set of subregions (or blocks) by prescribing the nodes contained in each subregion. Subregions are discussed in Section 3.2.2.

The block iterative logic contains a relaxation factor which can be used to under- or over-relax the solution and help damp or accelerate the rate of convergence. Implementation of the inner relaxation scheme is as follows:

$$C_i^{s+1} = (1 - o)C_i^s + oC_i^{s+1} \qquad (3\text{-}49)$$

where s denotes the inner iteration number and o is the relaxation factor. In general, the use of acceleration by over-relaxation ($1.0<o<1.9$) is appropriate for solutions of a diffusion-type equation, as generated in the hybrid formulation. For steady-state simulations where the advective-dispersive equation is utilized, under-relaxation ($0.5< o<1.0$) may be needed.

SECTION 4

DATA INPUT REQUIREMENTS

4.1 3DFEMWATER INPUT SEQUENCE

This section describes how to construct a data input file for 3DFEMWATER, the variably-saturated flow code. Background information about the code that will aid in building an input file, such as construction of a grid or selection of boundary condition types, is provided in Section 3.1. In addition, help in selecting values for some of the input parameters is given in Section 5.1.

Note that maximum control parameters are associated with a number of the input variables. These control parameters are used in the code to specify array dimensions. For some problems, the default values set for these parameters may be too small. If so, they can be easily changed. The maximum control parameters and their default values are listed in Appendix C. Note also that the logical units used by 3DFEMWATER are defined in Appendix B.

A complete input file consists of information supplied in 18 data sets. The contents and format of each data set are listed below. When constructing an input sequence, it is important to note that data sets 2 through 17 must be preceded by a record which contains a description of the data set. This can be seen in the example input sequences provided in Section 6.1. Most of the input is entered in free-format, which means that the spacing of the input data in a record does not need to follow a set pattern. Note that a record can consist of multiple lines, with a line defined as up to 80 columns.

The user may choose to run the model using any set of units as long as they are consistently maintained in all the input. Units of mass (M), length (L), and time (T) are indicated in the input descriptions.

4.1.1 Data Set 1: Title of the Simulation Run

One record with FORMAT(I5,A70,2X,I2,2I1) per problem. This record contains the following variables:

1. NPROB = Problem number (columns 1-5).

2. TITLE = Array for the title of the problem. It may contain up to 70 characters (columns 6- 75).

3. IGEOM = Integer indicating if (1) the geometry, boundary and pointer arrays are to be printed and if (2) the boundary and pointer arrays are to be computed or read via logical units (column 78). If IGEOM is an even number, geometry, boundary and pointer arrays will not be printed. If

IGEOM is an odd number, they will be printed. If IGEOM is less than or equal to 1, boundary arrays will be computed and written on logical unit LUBAR, but if IGEOM is greater than 1, boundary arrays will be read via logical unit LUBAR. If IGEOM is less than or equal to 3, pointer arrays will be computed and written on logical unit LUPAR, but if IGEOM is greater than 3, pointer arrays will be read via logical unit LUPAR. In summary:

IGEOM = Even No.	Print the geometry, boundary, and pointer arrays.
IGEOM = Odd No.	Do not print the arrays.
IGEOM ≤ 1	Compute and write boundary and pointer arrays.
$1 <$ IGEOM ≤ 3	Read boundary arrays, compute and write pointer arrays (not used under normal conditions).
IGEOM > 3	Read boundary and pointer arrays.

4. IBUG = Integer indicating if diagnostic output is desired to help determine problems encountered while executing the code (column 79);
   0 = no,
   1 = yes.

5. ICHNG = Integer control number indicating if the cyclic change of rainfall-seepage nodes is to be printed (column 80);
   0 = no,
   1 = yes.

4.1.2 Data Set 2: Basic Integer Parameters

One record with FREE-FORMAT per problem. It contains:

1. NNP = Number of nodal points. .

2. NEL = Number of elements.

3. NMAT = Number of material types.

4. NCM = Number of elements with material property correction.

5. NTI = Number of time steps or time increments (see notes at the end of Data Set 2).

6. KSS = Steady-state control;
   0 = steady-state solution,
   1 = transient-state solution (see note at the end of Data Set 2).

7. NMPPM = Number of material properties per material; this parameter should be set equal to 6 in the present version of the code (see Data Set 5).

8. KGRAV = Gravity term control;
   0 = no gravity term,
   1 = gravity term included.

9. ILUMP = Mass lumping control;
   0 = no,
   1 = yes.

10. IMID = Mid-difference control;
    0 = no,
    1 = yes.

11. NITER = Number of iterations allowed for solving the non-linear equation.

12. NCYL = Number of cycles permitted for iterating rainfall-seepage boundary conditions per time step.

13. NDTCHG = Number of times the time-step size will be reset to the initial time-step size; NDTCHG should be $\geq$ 1 (see Section 5.1.2.10).

14. NPITER = Number of iterations for a pointwise solution.

**** NOTE: NTI can be computed by NTI = 11 + 1 + 12 + 1, where 11 is the largest integer not exceeding Log(DELMAX/DELT)/Log(l+CHNG), 12 is the largest integer not exceeding (RTIME-DELT*((l+CHNG) **(I1+1)-1)/CHNG)/DELMAX, RTIME is the real simulation time, and DELMAX, DELT,and CHNG are defined in data set 3.

**** NOTE: A steady-state option may be used to provide either the final state of a system under study or the initial condition for a transient-state calculation. In the former case, KSS = 0 and NTI = 0 in this data set. In the latter case, KSS = 0 and NTI > 0. If KSS > 0, there will be no steady-state calculation.

4.1.3 Data Set 3: Basic Real Parameters

One record with FREE-FORMAT per problem. It contains:

1. DELT = Initial time step size, (T).

2. CHNG = Fractional change in the time-step size in each subsequent time increment, (dimensionless decimal-point value).

3. DELMAX = Maximum value of DELT, (T).

4. TMAX = Maximum simulation time, (T).

5. TOLA = Steady-state convergence criterion, (L).

6. TOLB = Transient-state convergence criterion, (L).

7. RHO = Density of water, (M/L^3).

8. GRAV = Acceleration of gravity, (L/T^2); (e.g., 32.17 ft/s^2 or 9.81 m/s^2).

9. VISC = Dynamic viscosity of water, (M/UT).

10. W = Time derivative weighting factor;
    0.5 = Crank-Nicolson central and/or mid-difference,
    1.0 = backward difference.

11. OME = Iteration parameter for solving the nonlinear matrix equation,
    0.0 < OME < 1.0 = under-relaxation,
    1.0 = exact relaxation,
    1.0 < OME < 2.0 = over-relaxation.

12. OMI = Relaxation parameter for solving the linearized matrix equation pointwise;
    0.0 < OMI < 1.0 = under relaxation,
    1.0 = exact relaxation,
    1.0 < OMI < 2.0 = over relaxation.

4.1.4 Data Set 4: Printer and Disk Storage Control and Times for Step Size Resetting

Three records are needed per problem. The first two records are formatted input with FORMAT(2I1). The third record is a FREE-FORMAT input. The number of lines for the first two records depends on the value of NTI, the number of time increments. The number of lines for the third record depends on the value of NDTCHG, the number of times to reset the time-step size.

Record 1 - FORMAT(2I1): This record contain the following variables:

1. KPR0 = Printer control for steady-state and initial conditions;
   0 = print nothing,
   1 = print the values for the variables FLOW, FRATE, and TFLOW,
   2 = print values above plus pressure head H,
   3 = print values above plus total head,
   4 = print values above plus moisture content,
   5 = print values above plus Darcy velocity.

2. KPR(I) = Printer control for the I-th (I = 1, 2, ... NTI) time step;
   0 = print nothing,
   1 = print the values for the variables FLOW, FRATE, and TFLOW,
   2 = print values above plus pressure head H,
   3 = print values above plus total head,
   4 = print values above plus moisture content,
   5 = print values above plus Darcy velocity.

Record 2 - FORMAT(2I1): This record can be used to store 3DFEMWATER output in a binary file for use in plotting or as input to 3DLEWASTE. It contains the following variables:

1. KDSK0 = Auxiliary storage control for the steady-state or initial condition;

   0 = no storage,
   1 = store on logical unit LUSTO.

2. KDSK(I) = Auxiliary storage control for the I-th (I = 1, 2, ... NTI) time step;

   0 = no storage,
   1 = store on logical unit LUSTO.

Record 3- FREE-FORMAT: This record contains the following variables:

1. TDTCH(I) = Time when the I-th (1 = 1, 2, ... NDTCHG) time-step-size resetting is needed.

4.1.5 Data Set 5: Material Properties

Either hydraulic conductivity or permeability can be input in this data set. The flag KCP in data set 6A is used to indicate which of the two is being used. A total of NMAT records are needed per problem, one for each material.

Record I (1 = 1, 2, ... NMAT) - FREE-FORMAT: Each record contains following variables:

1. PROP(1,I) = Saturated xx-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

2. PROP(2,I) = Saturated yy-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

3. PROP(3,I) = Saturated zz-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

4. PROP(4,I) = Saturated xy-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

5. PROP(5,I) = Saturated xz-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

6. PROP(6,I) = Saturated yz-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

4.1.6 Data Set 6: Soil Property Parameters

6A. Soil Property Control Integers

One record per problem. This record is FREE-FORMATTED and contains the following variables:

1. KSP = Soil property input control;
   0 = analytical input,
   1 = tabular data input.

2. NSPPM = Number of points in the tabular soil property functions when KSP = 1. The number of parameters needed to specify the analytical soil functions per material when KSP = 0. (For analytical soil functions, NSPPM = 5 in the current version of the code.)

3. KCP = Permeability input control;
   0 = input saturated hydraulic conductivity,
   1 = input saturated permeability.

6B. Analytical Soil Parameters

This subdata set is needed if and only if KSP = 0. NMAT records are needed, one for each material type.

Record I (I = 1, 2, ... NMAT) - FREE-FORMAT: Each record contains the following variables:

1. THPROP(1,I) = Residual moisture (water) content for material I, (--).

2. THPROP(2,I) = Saturated moisture (water) content for material I, (--).

3. THPROP(3,I) = Air entry pressure head for material I, (L).

4. THPROP(4,I) = Van Genuchten empirical coefficient alpha for material I, (1/L).

5. THPROP(5,I) = Van Genuchten empirical coefficient beta for material I, (--).

6C. Soil Properties in Tabular Form

This subdata set is needed if and only if KSP = 1. Four sets of records are needed -- one each for pressure, water-content, relative conductivity (or relative permeability), and water capacity, respectively. Each set contains NMAT records, one for each material type. Thus the total number of records for this subdata set is 4*NMAT. The number of lines in each record is determined by the input parameter NSPPM, defined in data set 6A.

Record I (I = 1, 2, ... NMAT) - FREE-FORMAT: Each record contains the following variables:

1. HPROP(1,I) = Tabular value of pressure head for the first data point of material I, (L).

2. HPROP(2,I) = Tabular value of pressure head for the second data point of material I, (L).

NSPPM. HPROP(NSPPM,I) = Tabular value of pressure head for the NSPPM-th data point of material I, (L).

Record (NMAT + I) (I = 1, 2, ... NMAT) - FREE-FORMAT: Each record contains the following variables:

1. THPROP(1,I) = Tabular value of moisture-content for the first data point in material I, (--).

2. THPROP(2,I) = Tabular value of moisture-content for the second data point in material 1, (--).

NSPPM. THPROP(NSPPM,I) = Tabular value of moisture-content for the NSPPM-th data point in material 1, (--).

Record (2*NMAT + I) (1 = 1, 2, ... NMAT) - FREE-FORMAT: Each record contains the following variables:

1. AKPROP(1,I) = Tabular value of relative conductivity for the first data point in material I, (--).

2. AKPROP(2,I) = Tabular value of relative conductivity for second data point in material I, (--).

NSPPM. AKPROP(NSPPM,I) = Tabular value of relative conductivity for the NSPPM-th data point in material I, (--).

Record (3*NMAT + I) (1 = 1, 2, ... NMAT) - FREE-FORMAT: Each record contains the following variables:

1. CAPROP(1,I) = Tabular value of moisture-content capacity for the first data point in material I, (1/L).

2. CAPROP(2,I) = Tabular value of moisture-content capacity for the second data point in material I, (1/L).

NSPPM. CAPROP(NSPPM,I) = Tabular value of moisture content capacity for the NSPPM-th data point in material I, (1/L).

4.1.7 Data Set 7: Nodal Point Coordinates

Coordinates for NNP nodes, specified in data set 2, are needed. Usually a total of NNP records are required. However, if a group of subsequent nodes appears in regular pattern, an automatic generation input option can be used.

Each record is FREE-FORMATTED and contains the following variables:

1. NI = Node number of the first node in the sequence.

2. NSEQ = NSEQ subsequent nodes will be automatically generated.

3. NAD = Increment of node number for each of the NSEQ subsequent nodes.
4. XNI = X-coordinate of node NI, (L).

5. YNI = Y-coordinate of node NI, (L).

6. ZNI = Z-coordinate of node NI, (L).

7. XAD = Increment of x-coordinate for each of the NSEQ subsequent nodes, (L).

8. YAD = Increment of y-coordinate for each of the NSEQ subsequent nodes, (L).

9. ZAD = Increment of z-coordinate for each of the NSEQ subsequent nodes, (L).

**** NOTE: A record with nine zeroes must be used to signal the end of this data set.

4.1.8 Data Set 8: Subregional Data

8A. Subregion Control Integer

One FREE-FORMATTED record is needed for this subdata set. It contains the following variable:

1. NREGN = Number of subregions.

8B. Number of Nodes in Each Subregion

Normally, NREGN records are required. However, if the sequence of node numbers follows a regular pattern between sequential subregions, the automatic generation input option can be used.

Each record is FREE-FORMATTED and contains the following five variables:

1. NK = Subregion number of the first subregion in a sequence.

2. NSEQ = Number of subsequent subregions which will be automatically generated.

3. NKAD = Increment of NK in each of the NSEQ subsequent subregions.

4. NODES = Number of nodes in the subregion NK.

5. NOAD = Increment of NODES in each of the NSEQ subsequent subregions.

**** NOTE: A record with five zeroes must be used to end the input of this subdata set.

8C. Mapping between Global Nodes and Subregion Nodes

This subdata set should be repeated NREGN times, once for each subregion. For each subregion, normally, the number of records equals the number of nodal points in the subregion. Automatic generation can be used, however, if the sequence of subregional node numbers follows a regular pattern.

Each record is FREE-FORMATTED and contains the following five variables:

1. LI = Local node number of the first node in a sequence.

2. NSEQ = Number of subsequent local nodes which will be generated automatically.

3. LIAD = Increment of LI for each of the NSEQ subsequent nodes.

4. NI = Global node number of local node LI.

5. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

**** NOTE: Local node numbers have values between one and the total number of nodes in a subregion (i.e., 1,2,.. ., NODES). Global node numbers are associated with the entire grid and are entered using data set 7.

4.1.9 Data Set 9: Element Incidence

Element incidence for NEL elements, specified in data set 2, are needed. Usually, a total of NEL records are needed. However, if a sequence of element numbers follows a regular pattern, the automatic generation input option can be used.

Each record is FREE-FORMATTED and contains the following variables:

1. MI = Global element number of the first element in a sequence.

2. NSEQ = Number of subsequent elements which will be automatically generated.

3. MIAD = Increment of MI for each of the NSEQ subsequent elements.

4. IE(MI,1) = Global node number of the first node of element MI.

5. IE(MI,2) = Global node number of the second node of element MI.

6. IE(MI,3) = Global node number of the third node of element MI.

7. IE(MI,4) = Global node number of the fourth node of element MI.

8. IE(MI,5) = Global node number of the fifth node of element MI.

9. IE(MI,6) = Global node number of the sixth node of element MI.

10. IE(MI,7) = Global node number of the seventh node of element MI.

11. IE(MI,8) = Global node number of the eighth node of element MI.

12. IEMAD = Increment of IE(MI,1) through IE(MI,8) for each of the NSEQ elements.

**** NOTE: IE(MI,1) - IE(MI,8) are numbered according to the convention shown in Figure 4.1. The first four nodes start from the front, lower, left corner and progress around the bottom element surface in a counterclockwise direction. The other four nodes begin from the front, upper, left corner and progress around the top element surface in a counterclockwise direction.

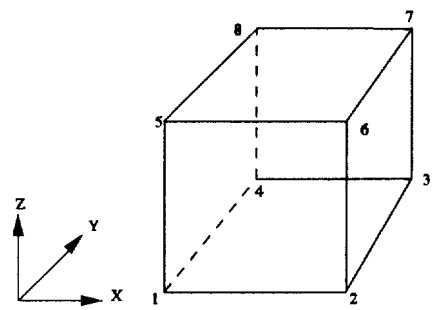


Figure 4.1. Node numbering convention for the elements.

4.1.10 Data Set 10: Material Type Correction

This data set is required only if NCM, defined in data set 2, is greater than zero. Normally, NCM records are required. However, if a group of element numbers follow a regular pattern, the automatic generation input option may be used.

Each record is FREE-FORMATTED and contains the following variables:

1. MI = Global element number of the first element in the sequence.

2. NSEQ = Number of subsequent elements which will be generated automatically.

3. MAD = Increment of element number for each of the NSEQ subsequent elements.

4. MITYP = Type of material for element MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent elements.

**** NOTE: A record with five zeroes must be used to signal the end of this data set.

4.1.11 Data Set 11: Card Input for Initial or Pre-Initial Conditions

NNP records (i.e., one record for each node) are normally needed. However, if a sequence of node numbers follows a regular pattern, automatic generation can be used.

Each record is FREE-FORMATTED and contains the following variables:

1. NI = Global node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NAD = Increment of node number for each of the NSEQ nodes.

4. HNI = Initial or pre-initial pressure head of node NI, (L).

5. HAD = Increment of initial or pre-initial head for each of the NSEQ nodes, (L).

6. HRD = Geometrical increment of HNI for each of the NSEQ subsequent nodes; (i.e, HNI**HRD).

**** NOTE: A record with six zeroes must be used to signal the end of this data set.

**** NOTE: The initial condition for a transient calculation may be obtained in two different ways: 1) it can be read directly from data set 11, or 2) the code can perform a steady-state simulation using time-invariant boundary conditions before automatically beginning the transient computations. For the first case, both KSS and NTI in data set 2 should be greater than zero. In the latter case, KSS = 0 and NTI > 0 and data set 11 is used to input the pre-initial condition, which is required as the starting condition for the steady-state iteration. In order to obtain a steady-state solution, both KSS and NTI are set equal to zero and data set 11 supplies the starting condition for the steady-state solution.

4.1.12 Data Set 12: Integer Parameters for Source and Boundary Conditions

One record per problem is needed. This record is FREE-FORMATTED and contains the following variables:

1. NSEL = Number of distributed source/sink elements.

2. NSPR = Number of distributed source/sink profiles (i.e., time histories).

3. NSDP = Number of data points in each of the NSPR source/sink profiles.

4. KSAI = Option for the distributed source/sink profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

5. NWNP = Number of well or point source/sink nodes.

6. NWPR = Number of well or point source/sink profiles (i.e., time histories).

7. NWDP = Number of data points in each of the NWPR profiles.

8. KWAI = Option for the well source/sink profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

9. NDNP = Number of fixed-head (Dirichlet) nodes (NDNP should be ≥ 1).

10. NDPR = Number of fixed-head profiles (i.e., time histories) (NDPR should be ≥ 1).

11. NDDP = Number of data points in each freed-head profile (NDDP should be ≥ 2).

12. KDAI = Option for the freed-head boundary value profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

13. NVES = Number of variable composite (rainfall/evaporation-seepage) boundary element sides.

14. NVNP = Number of variable composite boundary nodal points.

15. NRPR = Number of variable composite profiles (i.e., time histories).

16. NRDP = Number of data points in each of the NRPR profiles.

17. KRAI = Option for the variable composite profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

18. NCES = Number of specified-flux (Cauchy) boundary element sides.

19. NCNP = Number of specified-flux nodal points.

20. NCPR = Number of specfled-flux profiles (i.e., time histories).

21. NCDP = Number of data points in each of the NCPR profiles.

22. KCAI = Option for the specified-flux profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

23. NNES = Number of specified-pressure-head gradient (Neumann) boundary element sides.

24. NNNP = Number of specified-pressure-head gradient nodal points.

25. NNPR = Number of specified-pressure-head gradient flux profiles (i.e., time histories).

26. NNDP = Number of data points in each of the NNPR profiles.

27. KNAI = Option for the specified-pressure-head gradient profiles to be input analytically. This variable shouid be set equal to zero in the current version of the code.

4.1.13 Data Set 13: Distributed and Point Sources/Sinks

This data set is used to supply data for both distributed sources/sinks and well (point) sources/sinks.

13A. Distributed Sources/Sinks

The following three subdata sets are needed if and only if NSEL in data set 12 is greater than zero. The first subdata set is used to specify the distributed source/sink profiles. The second subdata set is used to read the global element numbers of the distributed source/sink elements. The third subdata set is used to assign a source/sink profile to each distributed source/sink element.

(a) Source/Sink Profiles

There will be NSPR (see data set 12) records in this subdata set. The number of lines in each record depends on the value of NSDP, defined in data set 12.

Record I (1 = 1, 2, ... NSPR) - FREE-FORMAT: Each record contains the following variables:

1. TSOSF(1,I) = Time of the first data point in the I-th profile, (T).

2. SOSF(1,I) = Source/sink value (as flux rate per unit volume of element) of the first data point in the I-th profile, ($L^3/T/L^2/L$); positive for a source and negative for a sink.

3. TSOSF(2,I) = Time of the second data point in the I-th profile, (T).

4. SOSF(2,I) = Source/sink value of the second data point in the I-th profile, ($L^3/T/L^2/L$); positive for a source and negative for a sink.

Up to NSDP data points.

(b) Global Element Number of All Distributed Source/Sink Elements

One record is needed for this subdata set. The number of lines in this record depends on NSEL, defined in data set 12. The record is FREE-FORMATTED and contains the following variables:

1. MSEL(1) = Global element number of the first distributed source/sink element.

2. MSEL(2) = Global element number of the second distributed source/sink element.

Up to NSEL numbers.

(c) Source/Sink Profile Type Assigned to Each Element

Usually NSEL records are needed. However, automatic generation can be used. Each record is FREE-FORMATTED and contains the following variables:

1. MI = Compressed element number of the first element in the sequence.

2. NSEQ = Number of elements which will be generated automatically.

3. MAD = Increment of element number for each of the NSEQ subsequent elements.

4. MITYP = Source/sink profile type associated with element ML

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent elements.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

**** NOTE: Compressed element numbers have values between one and the total number of distributed source/sink elements. Compressed element one corresponds to the first element listed in 13A(b), compressed element two corresponds to the second global element, etc.

13B. Point (Well) Source/Sink

The following three subdata sets are needed if and only if NWNP in data set 12 is greater than zero. The first subdata set is used to specify the point source/sink profiles. The second subdata set is used to read the global node numbers of the point source/sink nodes. The third subdata set is used to assign a source/sink profile to each point source/sink node.

(a) Source/Sink Profiles

There will be NWPR (see data set 12) records in this subdata set. The number of lines in each record depends on NWDP, defined in data set 12.

Record I (I = 1, 2, ... NWPR) - FREE-FORMAT: Each record contains the following variables:

1. TWSSF(1,I) = Time of the first data point in the I-th profile, (T).

2. WSSF(1,I) = Source/sink flow rate of the first data point in the I-th profile, (L^3/T); positive for a source and negative for a sink.

3. TWSSF(2,I) = Time of the second data point in the I-th profile, (T).

4. WSSF(2,I) = Source/sink flow rate of the second data point in the I-th profile, (L^3/T); positive for a source and negative for a sink.

Up to NWDP data points.

(b) Global Node Number of All Point (Well) Source/Sink Nodes

One record is needed for this subdata set. The number of lines in this record depends on NWNP, defined in data set 12. The record is FREE-FORMATTED and contains the following variables:

1. NPW(l) = Global node number of the first point source/sink node.

2. NPW(2) = Global node number of the second point source/sink node.

Up to NWNP numbers.

(c) Source/Sink Profile Type for Each Node

Usually NWNP records are needed. However, automatic generation can be used. Each record is FREE-FORMATTED and contains the following variables:

1. NI = Compressed point source/sink node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NAD = Increment of NI for each of the NSEQ subsequent nodes.

4. NITYP = Source/sink profile type associated with node NI.

5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.1.14 Data Set 14: Variable Composite (Rainfall/Evaporation-Seepage) Boundary Condition

The following six subdata sets are required if and only if NVES in data set 12 is greater than zero. The first subdata set is used to specify the rainfall/evaporation profiles. The second subdata set is used to assign the type of rainfall/evaporation profile to each of the variable composite boundary element sides. The third subdata set is used to specify the variable composite boundary element sides. The fourth subdata set is used to read the global nodal numbers of all the variable composite boundary nodes. The fifth subdata set is used to read the pending depth for each of the nodes. The sixth subdata set is used to read the allowed minimum pressure for each of the nodes.

14A. Rainfall/Evaporation-Seepage Profiles

There will be NRPR records (see data set 12) in this subdata set. The number of lines in each record depends on NRDP, defined in data set 12.

Record I (I = 1, 2, ... NRPR) - FREE-FORMAT: Each record contains the following variables:

1. TRF(1,I) = Time of the first data point in the I-th profile, (T).

2. RF(1,I) = Rainfall/evaporation rate of the first data point in the I-th profile, (L/T).

3. TRF(2,I) = Time of the second data point in the I-th profile, (T).

4. RF(2,I) = Rainfall/evaporation rate of the second data point in the I-th profile, (L/T).

Up to NRDP data points.

14B. Rainfall/Evaporation-Seepage Profile Type Assigned to Each Boundary Element Side

At most, NVES (see data set 12) records are needed. However, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed variable boundary element side number of the first element side in a sequence.

2. NSEQ = Number of subsequent variable boundary element sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent variable boundary element sides.

4. MITYP = Type of rainfall/evaporation-seepage profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

14C. Specification of Variable Composite Boundary Element Sides

Normally, NVES records are required, one each for a variable boundary element side. However, if a sequence of variable composite boundary element side numbers follows a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed variable boundary element side number of the first element side in a sequence.

2. NSEQ = Number of subsequent variable boundary element sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent variable boundary element sides.

4. I1 = Global node number of the first node of element side ML

5. I2 = Global node number of the second node of element side MI.

6. I3 = Global node number of the third node of element side MI.

7. I4 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of I1 for each of the NSEQ subsequent variable boundary element sides.

9. I2AD = Increment of I2 for each of the NSEQ subsequent variable boundary element sides.

10. I3AD = Increment of 13 for each of the NSEQ subsequent variable boundary element sides.

11. I4AD = Increment of 14 for each of the NSEQ subsequent variable boundary element sides.

**** NOTE: A record with 11 zeroes must be used to signal the end of this subdata set.

14D. Global Node Number of All Variable Composite Boundary Nodes

At most, NVNP records (see data set 12) are needed for this subdata set, one for each variable boundary node.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains five variables:

1. NI = Compressed variable boundary node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment of NI for each of the NSEQ nodes.

4. NODE = Global node number of node NI.

5. NODEAD = Increment of NODE for each of the NSEQ nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

14E. Pending Depth Allowed for Each Variable Composite Boundary Node

Normally, NVNP records (see data set 12) are needed. However, if a sequence of node numbers follows a regular pattern of pending depth, automatic generation is used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed variable boundary node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

4. HCONNI = Ponding depth of node NI, (L).

5. HCONAD = Increment of HCONNI for each of the NSEQ nodes, (L).

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

14F. Minimum Pressure Head Allowed for Each Variable Composite Boundary Node

Normally, NVNP records are needed. However, if a sequence of node numbers follows a regular pattern of minimum pressure head, automatic generation is used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed variable boundary node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

4. HMINNI = Minimum pressure head allowed for node NI, (L).

5. HMINAD = Increment of HMINNI for each of the NSEQ nodes, (L).

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.1.15 Data Set 15: Fixed-Head (Dirichlet) Boundary Condition

This data set is required only if NDNP in data set 12 is greater than zero. It consists of three subdata sets. The first subdata set is used to specify the fixed-head profiles. The second subdata set is used to read the global node numbers of the freed-head boundary nodes. The third subdata set is used to assign a head profile to each Dirichlet boundary node.

15A. Fixed-Head Profiles

There will be NDPR (see data set 12) records in this subdata set. The number of lines in each record depends on NDDP, the number of data points in each profile.

Record I (I = 1, 2, ... NDPR) - FREE-FORMAT: Each record contains the following variables:

1. THDBF(1,I) = Time of the first data point in the I-th profile, (T),

2. HDBF(1,I) = Total head of the first data point in the I-th profile, (L).

3. THDBF(2,I) = Time of the second data point in the I-th profile, (T).

4. HDBF(2,I) = Total head of the second data point in the I-th profile, (L).

Up to NDDP data points.

15B. Global Node Number of All the Dirichlet Nodes

One FREE-FORMATTED record is needed for this subdata set. The number of lines in this record depends on NDNP, defined in data set 12.

1. NPDB(1) = Global node number of the first compressed Dirichlet node.

2. NPDB(2) = Global node number of the second compressed Dirichlet node.

Up to NDNP numbers.

15C. Type of Head Profile Assigned to Each Fixed-Head Node

Normally one record per Dirichlet node (i.e., a total of NDNP records) is needed. However, if the Dirichlet node numbers follow a regular pattern, automatic generation may be used.

Record I (1 = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed Dirichlet node number of the first node in the sequence.

2. NSEQ = Number of subsequent Dirichlet nodes which will be generated automatically.

3. NIAD = Increment of NI for each of the NSEQ nodes.

4. NITYP = Type of total head profile assigned to node NI and NSEQ subsequent nodes.

5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.1.16 Data Set 16: Specified-Flux (Cauchy) Boundary Condition

This data set is required only if NCES in data set 12 is greater than zero. Four subdata sets are required. The first subdata set is used to read the specified-flux profiles. The second subdata set is used to read the type of specified-flux profile assigned to each of the specified-flux boundary element sides. The third subdata set is used to read the specified-flux boundary element sides. The fourth subdata set is used to read the global nodes associated with the specified-flux boundaries.

16A. Specified-Flux Profiles

There will be NCPR records (see data set 12) in this subdata set. The number of lines in each record depends on NCDP, defined in data set 12.

Record I (I = 1, 2, ... NCPR) - FREE-FORMAT: Each record contains the following variables:

1. TQCBF(1,I) = Time of the first data point in the I-th profile, (T).

2. QCBF(1,I) = Normal specified-flux of the first data point in the I-th profile, ($L^3/T/L^2$); positive out from the region, negative into the region.

3. TQCBF(2,I) = Time of the second data point in the I-th profile, (T).

4. QCBF(2,I) = Normal specified-flux of the second data point in the I-th profile, ($L^3/T/L^2$); positive out from the region, negative into the region.

Up to NCDP data points.

16B. Type of Specified-Flux Profile Assigned to Each Boundary Element Side

At most, NCES records (see data set 12) are needed. However, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-flux boundary element side number of the first side in the sequence.

2. NSEQ = Number of sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ sides.

4. MITYP = Type of specified-flux profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ sides.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

16C. Specified-Flux Boundary Element Sides

Normally, NCES records are required, one for each specified-flux boundary element side. However, if a group of specified-flux boundary element side numbers follows a regular pattern, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-flux boundary element side number of the first element side in a sequence.

2. NSEQ = Number of subsequent specified-flux element sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4. I1 = Global node number of the first node of element side MI.

5. I2 = Global node number of the second node of element side MI.

6. I3=Global node number of the third node of element side MI.

7. I4 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of I1 for each of the NSEQ subsequent element sides.

9. I2AD = Increment of I2 for each of the NSEQ subsequent element sides.

10. I3AD = Increment of I3 for each of the NSEQ subsequent element sides.

11. I4AD = Increment of I4 for each of the NSEQ subsequent element sides.

**** NOTE: A record with 11 zeroes must be used to end this subdata set.

16D. Global Node Number of All Compressed Specified-Flux Nodes

One FREE-FORMATTED record is needed for this subdata set. The number of lines in this record depends on NCNP, defined in data set 12.

1. NPCB(1) = Global node number of the first compressed specified-flux node.

2. NPCB(2) = Global node number of the second compressed specified-flux node.

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.

Up to NCNP numbers.

4.1.17 Data Set 17: Specified-Pressure-Head Gradient (Neumann) Boundary Condition

This data set is required if and only if NNNP in data set 12 is greater than zero. It consists of four subdata sets. The first subdata set is used to specify the specified-pressure-head gradient flux profiles. The second subdata set is used to assign a profile to each boundary element side. The third subdata set is used to read the global element sides of the specified-pressure-head gradient boundary elements. The fourth subdata set is used to read the global node numbers associated with the specified-pressure-head gradient boundaries.

17A. Prescribed Pressure-Head Gradient Flux Profiles

There will be NNPR records (see data set 12) in this subdata set. The number of lines in each record depends on NNDP, defined in data set 12.

Record I (I = 1, 2, ... NNPR) - FREE-FORMAT: Each record contains the following variables:

1. TQNBF(1,I) = Time of the first data point in the I-th profile, (T).

2. QNBF(1,I) = Normal specified-pressure-head gradient flux of the first data point in the I-th profile, ($L^3/T/L^2$); positive out from the region, negative into the region.

3. TQNBF(2,I) = Time of the second data point in the I-th profile, (T).

4. QNBF(2,I) = Normal specified-pressure-head gradient flux of the second data point in the I-th profile, ($L^3/T/L^2$); positive out from the region, negative into the region.

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.

Up to NNDP data points.

17B. Type of Specified-Pressure-Head Gradient Flux Profile Assigned to Each Boundary Element Side

At most, NNES records are needed (see data set 12). However, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-pressure-head gradient element side number of the first side in the sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ sides.

4. MITYP = Type of specified-pressure-head gradient flux profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ sides.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

17C. Specified-Pressure-Head Gradient Boundary Element Sides

Normally, NNES records are required, one for each specified-pressure-head gradient boundary element side. However, if a group of specified-pressure-head gradient boundary element side numbers follow a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-pressure-head gradient boundary element side number of the frost side in sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4. I1 = Global node number of the first node of element side MI.

5.0 I2 = Global node number of the second node of element side MI.

6. I3 = Global node number of the third node of element side MI.

7. I4 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of I1 for each of the NSEQ subsequent element sides.

9. I2AD = Increment of 12 for each of the NSEQ subsequent element sides.

10. I3AD = Increment of 13 for each of the NSEQ subsequent element sides.

11. I4AD = Increment of 14 for each of the NSEQ subsequent element sides.

**** NOTE: A record with 11 zeroes must be used to end this subdata set.

17D. Global Node Number of All Compressed Specified-Pressure-Head Gradient Nodes

One FREE-FORMATTED record is needed for this subdata set. The number of lines in this record depends on NNNP, defined in data set 12.

1. NPNB(1) = Global node number of the first compressed specified-pressure-head gradient node.

2. NPNB(2) = Global node number of the second compressed specified-pressure-head gradient node.

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Up to NNNP numbers.

4.1.18 Data Set 18: End of Job

If another problem is to be run, then input begins again with input data set 1. If termination of the job is desired, a blank line must be inserted at the end of the data set.

4.2 3DLEWASTE INPUT SEQUENCE

This section describes how to construct a data input file for 3DLEWASTE, the transport code. Background information about the code that will aid in building an input file, such as the types of adsorption isotherms allowed, is provided in Section 3.3. In addition, help in selecting values for some of the input parameters is given in Section 5.2.

Note that maximum control parameters are associated with a number of the input variables. These control parameters are used in the code to specify array dimensions. For some problems, the default values set for these parameters may be too small. If so, they can be easily changed. The maximum control parameters and their default values are listed in Appendix C. Note also that the logical units used by 3DLEWASTE are defined in Appendix B.

A complete input file consists of information supplied in 18 data sets. The contents and format of each data set are listed below. When constructing an input sequence, it is important to note that data sets 2 through 17 must be preceded by a record which contains a description of the data set. This can be seen in the example input sequences provided in Section 6.2. Most of the input is entered in free-format, which means that the spacing of the input data in a record does not need to follow a set pattern. Note that a record can consist of multiple lines, with a line defined as up to 80 columns.

The user may choose to run the model using any set of units as long as they are consistently maintained in all the input. Units of mass (M), length (L), and time (T) are indicated in the input descriptions.

4.2.1 Data Set 1: Title of the Simulation Run

One record with FORNLAT(I5,A70,3X,2I1) per problem. This record contains the following variables:

1. NPROB = Problem number (columns 1-5).

2. TITLE = Array for the title of the problem. It may contain up to 70 characters (columns 6- 75).

3. IGEOM = Integer indicating if (1) the geometry, boundary and pointer arrays are to be printed and if (2) the boundary and pointer arrays are to be computed or read via logical units (column 79). If IGEOM is an even number, geometry, boundary and pointer arrays will not be printed. If IGEOM is an odd number, they will be printed. If IGEOM is less than or equal to 1, boundary arrays will be computed and written on logical unit LUBAR, but if IGEOM is greater than 1, boundary arrays will be read via logical unit LUBAR. If IGEOM is less than or equal to 3, pointer arrays will be computed and written on logical unit LUPAR, but if IGEOM is greater than 3, pointer arrays will be read via logical unit LUPAR. In summary:

IGEOM = Even No.	Print the geometry, boundary, and pointer arrays.
IGEOM = Odd No.	Do not print the arrays.
IGEOM $\leq$ 1	Compute and write boundary and pointer arrays.
1 < IGEOM $\leq$ 3	Read boundary arrays, compute and write pointer arrays.
IGEOM > 3	Read boundary and pointer arrays.

4. IBUG = Integer indicating if diagnostic output is desired (column 80);
   0 = no,
   1 = yes.

4.2.2 Data Set 2: Basic Integer Parameters

One record with FREE-FORMAT per problem. It contains the following variables:

1. NNP = Number of nodal points.

2. NEL = Number of elements.

3. NMAT = Number of material types.

4. NCM = Number of elements with material property correction.

5. NTI = Number of time steps or time increments (see notes at the end of Data Set 2).

6. KSS = Steady-state control;
   0 = steady-state solution,
   1 = transient-state solution (see note at the end of Data Set 2).

7. NMPPM = Number of material properties per material; this parameter should be set equal to 8 in the present version of the code (see Data Set 5).

8. KVI = Velocity input control;
   -1 = velocity and moisture content read from data set 17,
   1 = steady-state velocity and moisture content input read from FEMWATER binary file,
   2 = transient velocity and moisture content input read from FEMWATER binary file.

9. ILUMP = Mass lumping control;
   0 = no,
   1 = yes.

10. IWET = Weighting function control;
    0 = Galerkin weighting,
    1 = upstream weighting.

11. IOPTIM = Optimization control;
    1 = upstream weighting optimization factor is to be computed,
    0 = factor is to be set equal to 1.0.

12. NITER = Number of iterations allowed for solving the non-linear equation.

13. NDTCHG = Number of times the time-step size will be reset to the initial time-step size; NDTCHG should be $\geq$ 1 (see Section 5.2.2.9).

14. NPITER = Number of iterations for a block or pointwise solution.

15. KSORP = Sorption model control;
    1 = linear isotherm,
    2 = Freundlich isotherm,
    3 = Langmuir isotherm.

**** NOTE: NTI can be computed by NTI = I1 + 1 + I2 + 1, where I1 is the largest integer not exceeding Log(DELMAX/DELT)/Log(1+CHNG), I2 is the largest integer not exceeding (RTIME-DELT*((1+ CHUG)** (I1+1)-1)/CHNG)/DELMAX, RTIME is the real simulation time, and DELMAX, DELT, and CHNG are defined in data set 3.

**** NOTE: A steady-state option may be used to provide either the final state of a system under study or the initial condition for a transient-state calculation. In the former case, KSS = 0 and NTI = 0 in this data set. In the latter case, KSS = 0 and NTI > 0. If KSS > 0, there will be no steady-state calculation.

4.2.3 Data Set 3: Basic Real Parameters

One record with FREE-FORMAT per problem. It contains the following variables:

1. DELT = Initial time step size, (T).

2. CHNG = Fractional change in the time-step size in each subsequent time increment, (dimensionless decimal-point value).

3. DELMAX = Maximum value of DELT, (T).

4. TMAX = Maximum simulation time, (T).

5. OME = Iteration parameter for solving the nonlinear matrix equation;
   0.0 < OME < 1.0 = under-relaxation,
   1.0 = exact relaxation,
   1.0 < OME < 2.0 = over-relaxation.

6. OMI = Relaxation parameter for solving the linearized matrix equation pointwise;
   0.0 < OMI < 1.0 = under relaxation,

1.0 = exact relaxation,
1.0 < OMI < 2.0 = over relaxation.

7. TOLB = Transient-state convergence criterion, (L).

8. TOLA = Steady-state convergence criterion, (L).

4.2.4 Data Set 4: Printer and Disk Storage Control and Times for Step Size Resetting

Three records are needed per problem. The first two records are formatted input with FORMAT(2I1). The third record is a FREE-FORMAT input. The number of lines for the first two records depends on the value of NTI, the number of time increments. The number of lines for the third record depends on the value of NDTCHG, the number of times to reset the time-step size.

Record 1 - FORMAT(2I1): This record contain the following variables:

1. KPR0 = Printer control for steady-state and initial conditions;
   0 = print nothing,
   1 = print values for the variables FLOW, FRATE, and TFLOW,
   2 = print values above plus concentration,
   3 = print values above plus material fluxes.

2. KFR(I) = Printer control for the I-th (I = 1, 2, ... NTI) time step; O = print nothing,
   1 = print values for the variables FLOW, FRATE, and TFLOW,
   2 = print values above plus concentration,
   3 = print values above plus material fluxes.

Record 2 - FORMAT(2I1): This record can be used to store 3DLEWASTE output in a binary file for use in plotting results. It contains the following variables:

1. KDSK0 = Auxiliary storage control for the steady-state or initial condition;

   0 = no storage,
   1 = store on logical unit LUSTO.

2. KDSK(I) = Auxiliary storage control for the I-th (I = 1, 2, ... NTI) time step;

   0 = no storage,
   1 = store on logical unit LUSTO.

Record 3- FREE-FORMAT: This record contains the following variables:

1. TDTCH(I) = Time when the I-th (I = 1, 2, ... NDTCHG) time-step-size resetting is needed.

4.2.5 Data Set 5: Material Properties

A total of NMAT records are required for this data set, one for each material.

Record I (I = 1, 2, ... NMAT) - FREE-FORMAT: Each record contains the following variables:

1. PROP(1,I) = Distribution coefficient (L^3/M) or Freundlich K or Langmuir K for medium I, depending on the value of KSORP in data set 2.

2. PROP(2,I) = Bulk density for medium I, (M/L^3).

3. PROP(3,I) = Longitudinal dispersivity for medium I, (L).

4. PROP(4,I) = Transverse dispersivity for medium I, (L).

5. PROP(5,I) = Molecular diffusion coefficient for medium I, (L^2/T).

6. PROP(6,I) = Tortuosity for medium I, (Dimensionless).

7. PROP(7,I) = Decay constant in medium I, (1/L).

8. PROP(8,I) = Freundlich N or Langmuir SMAX for medium I.

4.2.6 Data Set 6: Nodal Point Coordinates

Coordinates for NNP nodes are needed only if KVI $\leq$ 0, where NNP and KVI are defined in data set 2. Usually a total of NNP records are required. However, if a group of subsequent node numbers follows a regular pattern, an automatic generation input option can be used.

Each record contains the following variables and is FREE-FORMATTED.

1. NI = Node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be automatically generated.

3. NAD = Increment of node number for each of the NSEQ subsequent nodes.
4. XNI = X-coordinate of node NI, (L).

5. YNI = Y-coordinate of node NI, (L).

6. ZNI = Z-coordinate of node NI, (L).

7. XAD = Increment of x-coordinate for each of the NSEQ subsequent nodes, (L).

8. YAD = Increment of y-coordinate for each of the NSEQ subsequent nodes, (L).

9. ZAD = Increment of z-coordinate for each of the NSEQ subsequent nodes, (L).

**** NOTE: A record with nine zeroes must be used to signal the end of this data set.

4.2.7 Data Set 7: Element Incidence

Element incidence for NEL elements, specified in data set 2, are needed if $\leq$ O. Usually, a total of NEL records are needed. However, if a group of element numbers follows a regular pattern, the automatic generation input option can be used.

Each record is FREE-FORMATTED and contains the following variables:

1. MI = Global element number of the first element in a sequence.

2. NSEQ = Number of subsequent elements which will be automatically generated.

3. MIAD = Increment of MI for each of the NSEQ subsequent elements.

4. IE(MI,1) = Global node number of the first node of element MI.

5. IE(MI,2) = Global node number of the second node of element MI.

6. IE(MI,3) = Global node number of the third node of element MI.

7. IE(MI,4) = Global node number of the fourth node of element MI.

8. IE(MI,5) = Global node number of the fifth node of element MI.

9. IE(MI,6) = Global node number of the sixth node of element MI.

10. IE(MI,7) = Global node number of the seventh node of element MI.

11. IE(MI,8) = Global node number of the eighth node of element MI.

12. IEMAD = Increment of IE(MI,1) through IE(MI,8) for each of the NSEQ elements.

**** NOTE: IE(MI,1) - IE(MI,8) are numbered according to the convention shown in Figure 4.2. The first four nodes start from the front, lower, left corner and progress around the bottom element surface in a counterclockwise direction. The other four nodes begin from the front, upper, left corner and progress around the top element surface in a counterclockwise direction.

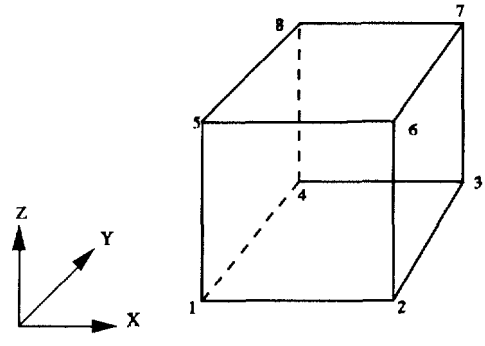

Figure 4.2. Node numbering convention for the elements.

4.2.8 Data Set 8: Subregional Data

This data set is needed only if KVI $\leq$ 0, where KVI is defined in data set 2.

8A. Subregion Control Integer

One FREE-FORMATTED record is needed for this subdata set. It contains the following variable:

1. NREGN = Number of subregions.

8B. Number of Nodes in Each Subregion

Normally, NREGN records are required. However, if the sequence of node numbers follows a regular pattern between sequential subregions, the automatic generation input option can be used.

Each record is FREE-FORMATTED and contains the following five variables:

1. NK = Subregion number of the first subregion in a sequence.

2. NSEQ = Number of subsequent subregions which will be automatically generated.

3. NKAD = Increment of NK in each of the NSEQ subsequent subregions.

4. NODES = Number of nodes in the subregion NK.

5. NOAD = Increment of NODES in each of the NSEQ subsequent subregions.

**** NOTE: A record with five zeroes must be used to end the input of this subdata set.

8C. Mapping between Global Nodes and Subregion Nodes

This subdata set should be repeated NREGN times, once for each subregion. For each subregion, normally, the number of records equals the number of nodal points in the subregion. Automatic generation can be used, however, if the subregional node numbers follow a regular pattern.

Each record contains five variables and is FREE-FORMATTED.

1. LI = Local node number of the first node in a sequence.

2. NSEQ = Number of subsequent local nodes which will be generated automatically.

3. LIAD = Increment of LI for each of the NSEQ subsequent nodes.

4. NI = Global node number of local node LI.

5. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

**** NOTE: Local node numbers have values between one and the total number of nodes in a subregion (i.e., 1,2,. ... NODES). Global node numbers are associated with the entire grid and are entered using data set 6.

4.2.9 Data Set 9: Material Type Correction

This data set is required only if NCM > 0 and KVI $\leq$ 0, where NCM and KVI are defined in data set 2. Normally, NCM records are required. However, if a group of element numbers follows a regular pattern, automatic generation may be used.

Each record is FREE-FORMATTED and contains the following variables:

1. MI = Global element number of the first element in the sequence.

2. NSEQ = Number of subsequent elements which will be generated automatically.

3. MAD = Increment of element number for each of the NSEQ subsequent elements.

4. MITYP = Type of material for element MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent elements.

**** NOTE: A record with five zeroes must be used to signal the end of this data set.

4.2.10 Data Set 10: Card Input for Initial or Pre-Initial Conditions

NNP records (i.e., one record for each node) are normally needed. However, if a group of node numbers follow a regular pattern, automatic generation can be used.

Each record is FREE-FORMATTED and contains the following variables:

1. NI = Global node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NAD = Increment of node number for each of the NSEQ nodes.

4. CNI = Initial or pre-initial concentration of node NI, (M/L^3).

5. CAD = Increment of CNI for each of the NSEQ nodes, (M/L^3).

6. CRD = Geometrical increment of CNI for each of the NSEQ subsequent nodes (i.e, CNI**CRD).

**** NOTE: A record with six zeroes must be used to signal the end of this data set.

**** NOTE: The initial condition for a transient calculation may be obtained in two different ways: 1) it can be read directly from data set 10, or 2) the code can perform a steady-state simulation using time-invariant boundary conditions before beginning the transient computations. For the first case, both KSS and NTI in data set 2 should be greater than zero. In the latter case, KSS = 0 and NTI > 0 and data set 10 is used to input the pre-initial condition, which is required as the starting condition for the steady-state iteration. In order to obtain a steady-state solution, both KSS and NTI are set equal to zero and data set 11 supplies the starting condition for the steady-state solution.

4.2.11 Data Set 11: Integer Parameters for Sources and Boundary Conditions

One record per problem is needed. This record is FREE-FORMATTED and contains the following variables:

1. NSEL = Number of distributed source/sink elements.

2. NSPR = Number of distributed source/sink profiles (i.e., time histories) (NSPR should be $\geq$ 1).

3. NSDP = Number of data points in each of the NSPR source/sink profiles (NSDP should be $\geq$ 2).

4. KSAI = Option for the distributed source/sink profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

5. NWNP = Number of well or point source/sink nodes.

6. NWPR = Number of well or point source/sink profiles (i.e., time histories).

7. NWDP = Number of data points in each of the NWPR profiles.

8. KWAI = Option for the well source/sink profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

9. NDNP = Number of prescribed-concentration (Dirichlet) nodes (NDNP should be $\geq$ 1).

10. NDPR = Number of prescribed-concentration profiles (i.e., time histories) (NDPR should be $\geq$ 1).

11. NDDP = Number of data points in each prescribed-concentration profile (NDDP should be $\geq$ 2).

12. KDAI = Option for the prescribed-concentration boundary profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

13. NVES = Number of variable composite boundary element sides.

14. NVNP = Number of variable composite boundary nodal points.

15. NRPR = Number of variable composite profiles (i.e., time histories).

16. NRDP = Number of data points in each of the NRPR profiles.

17. KRAI = Option for the variable composite profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

18. NCES = Number of specified-flux (Cauchy) boundary element sides.

19. NCNP = Number of specified-flux boundary nodal points.

20. NCPR = Number of specified-flux profiles (i.e., time histories).

21. NCDP = Number of data points in each of the NCPR profiles.

22. KCAI = Option for the specified-flux profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

23. NNES = Number of specified-dispersive-flux (Neumann) boundary element sides.

24. NNNP = Number of specified-dispersive-flux boundary nodal points.

25. NNPR = Number of specified-dispersive-flux profiles (i.e., time histories).

26. NNDP = Number of data points in each of the NNPR profiles.

27. KNAI = Option for the specified-dispersive-flux profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

4.2.12 Data Set 12: Distributed and Point Sources/Sinks

This data set is used to supply data for both distributed sources/sinks, and point (well) sources/sinks.

12A. Distributed Sources/Sinks

The following three subdata sets are needed if and only if NSEL in data set 11 is greater than zero. The first subdata set is used to specify the distributed source/sink profiles. The second subdata set is used to read the global element numbers of the distributed source/sink elements. The third subdata set is used to assign a source/sink profile to each distributed source/sink element.

(a) Sources/Sink Profiles

NSPR records (see data set 11) are needed. Each record contains NSDP data points, defined in data set 11. Three numbers, representing the time, source flow rate, and source concentration, respectively, are associated with each data point.

Record I (I = 1, 2, ... NSPR) - FREE FORMAT: Each record contains the following variables:

1. TSOSF(J,I) = Time of J-th data point in I-th profile, (T).

2. SOSF(J,I,1) = Source/sink flow rate of the J-th data point in the I-th profile, (L^3/WL^3); positive for source and negative for sink.

3. SOSF(J,I,2) = Source/sink concentration of the J-th data point in the I-th profile, (M/L^3).

.
.

Up to NSDP data points.

(b) Global Element Number of All Distributed Source/Sink Elements

One record is needed for this subdata set. The number of lines in the record depends on NSEL, defined in data set 11. The record is FREE-FORMATTED and contains the following variables:

1. LES(1) = Global element number of the first distributed source/sink element.

2. LES(2) = Global element number of the second distributed source/sink element.

   .
   .

   Up to NSEL numbers.

(c) Source/Sink Profile Type Assigned to Each Element

Usually NSEL records are needed. However, automatic generation can be used. Each record is FREE-FORMATTED and contains the following variables:

1. MI = Compressed element number of the first element in the sequence.

2. NSEQ = Number of subsequent elements which will be automatically generated.

3. MAD = Increment of element number for each of the NSEQ elements.

4. MITYP = Source/sink profile associated with element MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent elements.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

**** NOTE: Compressed element numbers have values between one and the total number of distributed source/sink elements. Compressed element one corresponds to the first element listed in 12A(b), compressed element two corresponds to the second global element, etc.

12B. Point (Well) Source/Sink

The following three subdata sets are needed only if NWNP in data set 11 is greater than zero. The first subdata set is used to specify the point source/sink profiles. The second subdata set reads the source/sink global node numbers, and the third assigns a source/sink profile type to each node.

(a) Source/Sink Profiles

NWPR records (see data set 11) are needed. Each record contains NWDP data points, defined in data set 11. Three numbers, representing the time, source flow rate, and source concentration, respectively, are associated with each data point.

Record I (I = 1, 2, ... NWPR) - FREE FORMAT: Each record contains the following variables:

1. TWSSF(J,I) = Time of J-th data point in I-th profile, (T).

2. WSSF(J,I,1) = Source/sink flow rate of the J-th data point in the I-th profile, (L^3/T); positive for source and negative for sink.

3. WSSF(J,I,2) = Source/sink concentration of the J-th data point in the I-th profile, (M/L^3).

.
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Up to NWDP numbers.

(b) Global Node Number of All Point (Well) Source/Sink Nodes

One record is needed for this subdata set. The number of lines in this record depends on NWNP, defined in data set 11. The record is FREE-FORMATTED and contains the following variables:

1. NPW(1) = Global node number of the first point source/sink node.

2. NPW(2) = Global node number of the second point source/sink node.

.
.

Up to NWNP numbers.

(c) Source/Sink Profile Type for Each Node

Usually one record per node (i.e., NWNP records) are needed. However, automatic generation can be used. Each record is FREE-FORMATTED and contains the following variables:

1. NI = Compressed point source/sink node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be automatically generated.

3. NIAD = Increment of NI for each of the NSEQ nodes.

4. NITYP = Source/sink profile associated with node NI.

5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

****NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.2.13 Data Set 13: Variable Composite Boundary Condition

The following four subdata sets are required only if NVES in data set 11 is greater than zero. The first subdata set is used to specify the concentration profiles. The second subdata set is used to assign a concentration profile type to each of the variable composite boundary element sides. The third subdata set is used to specify the variable composite boundary element sides. The fourth subdata set is used to read the global nodal number of all the variable composite boundary nodes.

13A. Concentration Profiles

There will be NRPR records (see data set 11) in this subdata set. The number of lines in each record depends on NRDP, defined in data set 11.

Record I (I = 1, 2, ... NRPR) - FREE-FORMAT: Each record contains the following variables:

1. TCRSF(1,I) = Time of the first data point in the I-th profile, (T).

2. CRSF(1,I) = Concentration of the first data point in the I-th profile, (M/L^3).

3. TCRSF(2,I) = Time of the second data point in the I-th profile, (T).

4. CRSF(2,I) = Concentration of the second data point in the I-th profile, (M/L^3).

Up to NRDP data points.

13B. Concentration Profile Type Assigned to Each Boundary Element Side

Usually one record per variable composite boundary element side is needed. However, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed variable boundary element side of the first side in a sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MJAD = Increment of MI for each of the NSEQ subsequent sides.

4. MITYP = Type of concentration profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

****NOTE: A record with five zeroes must be used to signal the end of this subdata set.

13C. Specification of Variable Composite Boundary Element Sides

Normally, NVES records are required, one each for a variable boundary element side. However, if a group of variable composite boundary element sides appears in a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed variable composite boundary element side number of the first side in a sequence.

2. NSEQ = Number of subsequent element sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ element sides.

4. 11 = Global node number of the first node of element side MI.

5. 12 = Global node number of the second node of element side MI.

6. 13 = Global node number of the third node of element side MI.

7. 14 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of 11 for each of the NSEQ subsequent element sides.

9. I2AD = Increment of 12 for each of the NSEQ subsequent element sides.

10. 13AD = Increment of 13 for each of the NSEQ subsequent element sides.

11. I4AD = Increment of 14 for each of the NSEQ subsequent element sides.

****NOTE: A record with 11 zeroes must be used to signal the end of this subdata set.

13D. Global Nodal Number of All Variable Composite Boundary Nodes

At most, NVNP records (see data set 11) are needed for this subdata set.
Record I (1 = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed variable boundary node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment for NI for each of the NSEQ nodes.

4. NODE = Global nodal number of the node NI.

5. NODEAD = Increment of NODE for each of the NSEQ subsequent nodes.

****NOTE: A record with five zeroes must be used to signal end of this subdata set.

4.2.14 Data Set 14: Prescribed-Concentration (Dirichlet) Boundary Condition

This data set is required if and only if NDNP in data set 11 is greater than zero. It consists of three subdata sets. The first subdata set is used to specify the prescribed-concentration profiles, the second is used to read the prescribed-concentration boundary nodes, and the third is used to assign a concentration profile type to each of the Dirichlet nodes.

14A. Prescribed-Concentration Profiles

There will be NDPR records (see data set 11) in this subdata set. The number of lines in each record depends on NDDP, defined in data set 11.

Record I (I = 1, 2, ... NDPR) - FREE-FORMAT: Each record contains the following variables:

1. TCDBF(l,I) = Time of first data point in I-th profile, (T).

2. CDBF(1,I) = Concentration of first data point in I-th profile, (M/L^3).

3. TCDBF(2,I) = Time of second data point in I-th profile, (T).

4. CDBF(2,I) = Concentration of second data point in I-th profile, (M/L^3).

Up to NDDP data points.

14B. Global Node Number of All the Prescribed-Concentration Nodes

One FREE-FORMATTED record is needed for this subdata set. The number of lines in this record depends on NDNP, defined in data set 11.

1. NPDB(l) = Global node number of the first compressed prescribed-concentration node.

2. NPDB(2) = Global node number of the second compressed prescribed-concentration node.

Up to NDNP numbers.

14C. Type of Concentration Profile Assigned to Each Dirichlet Node

Normally one record per Dirichlet node (i.e., a total of NDNP records) is needed. However, if the Dirichlet node numbers follow a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed Dirichlet node number of the first node in the sequence.

2. NSEQ = Number of subsequent Dirichlet nodes which will be automatically generated.

3. NIAD = Increment of NI for each of the NSEQ nodes.

4. NITYP = Dirichlet concentration profile type assigned to node NI and NSEQ subsequent nodes.

5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

****NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.2.15 Data Set 15: Specified-Flux (Cauchy) Boundary Condition

Four subdata sets are required only if NCES in data set 11 is greater than zero. The first subdata set is used to read the specified-flux profiles. The second subdata set is used to assign the type of specified-flux profile to each of the specified-flux boundary element sides. The third subdata set is used to read the specified-flux boundary element sides. The fourth subdata set is used to read the global nodal numbers associated with the specified-flux boundaries.

15A. Specified-Flux Profiles

There will be NCPR records (see data set 11) in this subdata set. The number of lines in each record depends on NCDP, defined in data set 11.

Record I (I = 1, 2, ... NCPR) - FREE-FORMAT: Each record contains the following variables:

1. TQCBF(1,I) = Time of the first data point in the I-th profile, (T).

2. QCBF(l,I) = Normal specified-flux of the first data point in the I-th profile, ($M/T/L^2$); positive out of the region, negative into the region.

3. TQCBF(2,I) = Time of the second data point in the I-th profile, (T).

4. QCBF(2,I) = Normal specified-flux of the second data point in the I-th profile, ($M/T/L^2$); positive out of the region, negative into the region.

Up to NCDP data points.

15B. Type of Specified-Flux Profile Assigned to Each Boundary Element Side

At most, NCES records (see data set 11) are needed. However, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-flux boundary element side number of the first side in the sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of NSEQ subsequent sides.

4. MITYP = Type of specified-flux profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

****NOTE: A record with five zeroes must be used to signal the end of this subdata set.

15C. Specified-Flux Boundary Element Sides

Normally, NCES records are required, one for each specified-flux boundary element side. However, if a group of specified-flux boundary element side numbers follows a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-flux boundary element side number of the first element side in a sequence.

2. NSEQ = Number of subsequent element sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4. 11 = Global node number of the first node of element side MI.

5. 12 = Global node number of the second node of element side MI.

6. 13 = Global node number of the third node of element side MI.

7. 14 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of 11 for each of the NSEQ subsequent element sides.

9. I2AD = Increment of 12 for each of the NSEQ subsequent element sides.

10. I3AD = Increment of 13 for each of the NSEQ subsequent element sides.

11. I4AD = Increment of 14 for each of the NSEQ subsequent element sides.

****NOTE: A record with 11 zeroes must be used to signal the end of this subdata set.

15D. Global Node Number of All Compressed Specified-Flux Boundary Nodes

Usually NCNP records (see data set 11) are needed for this subdata set. However, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed specified-flux boundary node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment for NI for each of the NSEQ nodes.

4. NODE = Global nodal number of the node NI.

5. NODEAD = Increment of the global nodal number for each of the NSEQ subsequent nodes.

****NOTE: A record with five zeroes must be used to signal end of this subdata set.

4.2.16 Data Set 16: Specified-Dispersive-Flux (Neumann) Boundary Condition

The following four subdata sets are required only if NNES in data set 11 is greater than zero. The first subdata set is used to read the specified-dispersive-flux profiles. The second subdata set is used to assign a specified-dispersive-flux profile type to each boundary element sides. The third subdata set is used to read the specified-dispersive-flux boundary element side. The fourth subdata set is used to read the global nodal numbers associated with the specfied-dispersive-flux boundaries.

16A. Prescribed Specified-Dispersive-Flux Profiles

There will be NNPR records (see data set 11) in this subdata set. The number of lines in each record depends on NNDP, defined in data set 11.

Record I (I = 1, 2, ... NNPR) - FREE-FORMAT: Each record contains the following variables:

1. TQNBF(l,I) = Time of the first data point in the I-th profile, (T).

2. QNBF(l,I) = Normal specified-dispersive flux of the first data point in the I-th profile, $(M/T/L^2)$; positive out of the region, negative into the region.

3. TQNBF(2,I) = Time of the second data point in the I-th profile, (T).

4. QNBF(2,I) = Normal specified-dispersive flux of the second data point in the I-th profile, $(M/T/L^2)$; positive out of the region, negative into the region.

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Up to NNDP data points.

16B. Type of Specified-Dispersive-Flux Profile Assigned to Each Boundary Element Side

At most, NNES records (see data set 11) are needed. However, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-dispersive-flux boundary element side of the first side in a sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of NSEQ subsequent sides.

4. MITYP = Type of specified-dispersive-flux profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

****NOTE: A record with five zeroes must be used to signal the end of this subdata set.

16C. Specified-Dispersive-Flux Boundary Element Sides

Normally, NNES records are required, one for each specified-dispersive-flux boundary element side. However, if a group of specified-dispersive-flux element side numbers follows a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-dispersive-flux boundary element side number of the first element side in a sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4. I1 = Global node number of the first node of element side MI.

5. 12 = Global node number of the second node of element side MI.

6. 13 = Global node number of the third node of element side ML

7. 14 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of 11 for each of the NSEQ subsequent element sides.

9. I2AD = Increment of 12 for each of the NSEQ subsequent element sides.

10. I3AD = Increment of 13 for each of the NSEQ subsequent element sides.

11. I4AD = Increment of 14 for each of the NSEQ subsequent element sides.

****NOTE: A record with 11 zeroes must be used to signal the end of this subdata set.

16D. Global Node Number of All Compressed Specified-Dispersive-Flux Boundary Nodes

Usually NNNP records (see data set 11) are needed for this subdata set. However, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed specified-dispersive-flux boundary node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment of NI for each of the NSEQ nodes.

4. NODE = Global nodal number of the node NI.

5. NODEAD = Increment of the global nodal number for each of the NSEQ subsequent nodes.

****NOTE: A record with five zeroes must be used to signal end of this subdata set.

4.2.17 Data Set 17: Hydrological Variables

This data set is needed only if KVI in data set 2 is less than or equal to zero. When KVI $\leq$ 0, two subdata sets are needed: one for the velocity field and the other for the moisture content.

17A. Velocity Field

Usually NNP records (see data set 2) are needed. However, if the velocity values follow a regular pattern, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. NI = Node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be automatically generated.

3. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

4. VXNI = X-velocity component at node NI, (L/T).

5. VYNI = Y-velocity component at node NI, (L/T).

6. VZNI = Z-velocity component at node NI, (L/T).

7. VXAD = Increment of VXNI for each of the NSEQ subsequent nodes, (L/T).

8. VYAD = Increment of VYNI for each of the NSEQ subsequent nodes, (m).

9. VZAD = Increment of VZNI for each of the NSEQ subsequent nodes, (m).

****NOTE: A record with nine zeroes must be used to signal the end of this subdata set.

17B. Moisture Content Field

Usually, NEL records (see data set 2) are needed. However, if the moisture content values follow a regular pattern, automatic generation can be used.

Record I (I = 1, 2, ...) - FREE-FORMAT: Each record contains the following variables:

1. MI = Element number of the first element in a sequence.

2. NSEQ = Number of subsequent elements which will be automatically generated.

3. MIAD = Increment of MI for each of NSEQ subsequent elements.

4. THNI = Moisture content of element MI, (decimal point).

5. THNIAD = Increment of THNI for the NSEQ subsequent elements, (decimal point).

****NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.2.18 Data Set 18: End of Job

If another problem is to be run, then input begins again with input data set 1. If termination of the job is desired, a blank line must be inserted at the end of the data set.

SECTION 5

PARAMETER SELECTION

This section provides guidance in selecting values for some of the parameters required as input to the 3DFEMWATER/3DLEWASTE codes. This guidance is not intended in any way to be used as a substitute for data collection. The most accurate model results are obtained from simulations which are based on site-specific information. In some cases, however, it is not feasible to measure certain parameters, and satisfactory results may be obtained using estimated values taken from the reported ranges presented here.

For easy reference, the parameters are grouped according to the data group in which they appear in the input data sets (see Section 4). Concepts, such as initial and boundary conditions, isotherms, distributed and point sources and sinks, and subregional data, were introduced in Section 3 and guidance is not provided in this section for related parameters.

5.1 3DFEMWATER

5.1.1 Data Set 1: Title of the Simulation Run

5.1.1.1 Geometry, Boundary, and Pointer Array Control, IGEOM [--]

The integer IGEOM has two functions. It is used to specify if geometry, boundary, and pointer arrays should be printed so that the user can examine them. It also controls whether the boundary and pointer arrays are written to or read from binary files. Boundary arrays store data related to the boundary conditions. Pointer arrays store the global matrix in compressed form and are used to construct the subregional block matrices. For large problems, it takes too much time to generate these arrays for each computer execution of a particular scenario. Usually, they should be generated only once and stored in binary files using logical units LUBAR and LUPAR (see Table B-l).

In order to compute and store the boundary and pointer arrays, the user should choose a value for IGEOM less than or equal to one. In subsequent runs, the boundary and pointer arrays can be read from the binary files by changing the value of IGEOM to a number greater than three. Whenever changes are made to the model which involve the geometry of the problem, the boundary conditions, and the configuration of the subregions, the arrays must be generated and stored again. Note that the option presented in the input to read boundary arrays and compute and write pointer arrays is not used in 3DFEMWATER under normal conditions.

For the options explained above, if the number chosen by the user is even, the arrays will be printed as output. If the number is odd, the arrays will not be printed.

5.1.2 Data Set 2: Basic Integer Parameters

5.1.2.1 Number of Material Types, NMAT [--]

This parameter is the total number of different porous media being modeled. For example, if the region of interest is predominantly sand with clay lenses, then the value of NMAT should be set equal to two. When material properties are assigned to each material type, using data set 5 (see Section 4.1.5), the first material type should be the predominant porous medium (e.g., for the example here, the sand).

5.1.2.2 Number of Elements with Material Property Correction, NCM [--]

In the code, all the grid elements automatically are initialized as having a material type of one. If the region being modelled is homogeneous, the parameter NCM is set equal to zero. To model a heterogeneous porous medium, NCM and the parameters in data set 10 of the input (see Section 4.1.10) are used to specify which elements have different material types associated with them. The parameter NCM is the total number of elements which have a material type different than the first material type.

5.1.2.3 Number of Time-Steps, NTI [--]

For a constant time-step size, this number is obtained by dividing the simulation time by the time-step size, DELT. If the time-step size is variable, this number is computed using the formula given in the note at the end of data set 2 in Section 4.1.2. If a steady-state solution is desired, NTI should be set equal to zero.

5.1.2.4 Steady-State Control, KSS [--]

As noted in Section 4.1.2, a steady-state option may be used to provide either the final state of a system under study or the initial condition for a transient-state calculation. In the former case, both KSS and the number of time steps, NTI, should be set to zero. In the latter case (i.e., when KSS = 0 and NTI > 0), the code performs a steady-state calculation before beginning the transient computations. If KSS = 1, no steady-state calculation is performed. Rather, the code begins transient calculations using initial conditions supplied in data set 11 of the input.

5.1.2.5 Gravity Term Control, KGRAV [--]

This parameter indicates if the gravity term should be included. For most cases, KGRAV should be equal to 1. For cases when flow due to the pressure gradient is much greater than that due to gravity, KGRAV is set to 0.

5.1.2.6 Mass Lumping Flag, ILUMP [--]

This parameter indicates if the mass matrix is to be lumped or not. Normally, one should set this parameter to O. Without lumping, the solution is more accurate. However, for occasions when negative concentrations or oscillating solutions occur, this parameter should be set to 1. It has been suggested that for saturated-unsaturated flow computations, the parameter ILUMP should always be set equal to 1.

5.1.2.7 Mid-differencing Flag, IMID [--]

This parameter indicates if the more accurate mid-difference method should be used in flow computations. For practical purposes, IMID = 0 should be sufficient. IMID = 1 is used only for research purposes.

5.1.2.8 Number of Iterations for the Nonlinear Equation, NITER [--]

This parameter is the number of iterations allowed for solving the nonlinear equation. Normally, NITER = 50 should be sufficient. If this number is exceeded and the solution does not converge, the program will issue a warning message. When this occurs, the user should first recheck the input values. If the input is correct, the program can be re-executed using a larger value for NITER.

5.1.2.9 Number of Cycles, NCYL [--]

This parameter indicates how many cycles are used for iterating the boundary conditions. A value of 20 should be adequate for most problems.

5.1.2.10 Number of Times to Reset the Time Step, NDTCHG [--]

This parameter indicates how many times the time-step size should be reset to the initially small time-step size. When we start a simulation, we normally use a small time-step size. However, for every consecutive time step, we may gradually increase the time-step size by some amount specified by the variable CHNG in Data Set 3 in Section 4.1.3. When a steep change in boundary conditions or source/sink conditions occurs, however, the time-step size should be reset to the initially small value. (See the example problem in Section 6.1.1.) NDTCHG tells us how many times we want to reset the time-step size during a simulation.

The value of NDTCHG must be at least one. If the user does not want to reset the time step, a value of one should be entered here and a very large number, larger than the total simulation time, should be entered for TDTCH(l) in data set 4 (see Section 4.1.4).

5.1.2.11 Number of Iterations for Pointwise Solution, NPITER [--]

This parameter is used to input the number of iterations allowed for solving the matrix equations with the block iteration method. A value of 300 should be sufficient for most problems. If this number is exceeded and the solution does not converge, the program will issue a warning message. When this occurs, the users should re-execute the program using a larger value for NPITER.

5.1.3 Data Set 3: Basic Real Parameters

5.1.3.1 Initial Time-Step Size, DELT [T]

This is the time-step size used for the first time-step computation if the variable CHNG is not equal to 0.0. It is the time-step size used for every time step if the variable CHNG is set equal to 0.0. It is advisable to choose the value of DELT such that:

$$(F*DELX*DELX)/(DELT*K) \leq 1$$

where

DELX = the element size (L)
K = hydraulic conductivity (L/T)
F = specific storage (l/L)

For example, if F = 0.001 l/m, K = 0.00001 m/sec, and an element size of 10 m is used, then DELT should be less than 10,000 seconds.

5.1.3.2 Fractional Change in Time-Step Size, CHNG [--]

This parameter specifies how much of an increase one would like to make to the time-step size for each subsequent time step. Normally, a value from 0.0 to 0.5 can be used.

5.1.3.3 Maximum Allowable Time Step, DELMAX [T]

The maximum time-step size allowed depends on how fast the system responds to change. Use of a value one to ten times the size of the initial time step is advised.

5.1.3.4 Maximum Simulation Time, TMAX [T]

This is the actual length of time to be simulated. If this time is exceeded before you have made NTI step computations, the simulation will be terminated.

5.1.3.5 Steady-State Convergence Criterion, TOLA [L]

This is the absolute error allowed for assessing if a steady-state solution for hydraulic head has converged. The value used for TOLA depends on how much the system is disturbed. Normally, setting TOLA equal to one-ten-thousandth (0.0001) of the maximum disturbance should be sufficient. For example, if one is conducting a simulation of drawdown due to pumping and one expects the maximum drawdown at steady-state will be 1 m, then a value of TOLA equal to 0.0001 m should be sufficient.

5.1.3.6 Transient Convergence Criterion, TOLB [L]

This is the absolute error allowed for assessing if the solution for hydraulic heads has converged for each transient time step. A value equal to one-hundred-thousandth (0.00001) of the maximum disturbance should be sufficient for most problems.

5.1.3.7 Density of Water, RHO [M/L^3]

The density of water, ρ_w, is the ratio of its mass to its volume and has SI units of kg/m^3. Density varies with temperature (Table 5-1) and can be computed using regression equations presented in CRC (1981). Density also varies with the concentration of dissolved chemical species. Water density appears in the definition of specific storage

TABLE 5-1. WATER DENSITY AS A FUNCTION OF TEMPERATURE

Temperature (°C)	Density (kg/m^3)
0	999.87
10	999.73
20	998.23
30	995.67
40	992.24
50	988.07
60	983.24
70	977.81
80	971.83
90	965.34
100	958.38

Source: Mercer et al., 1982; Original Reference: CRC, 1965

and in the relationship between hydraulic conductivity and intrinsic permeability (Section 5.1.4.2).

5.1.3.8 Dynamic Viscosity of Water, VISC [M/L/T]

The viscosity of a fluid is a measure of the forces that work against flow when a shearing stress is applied (Lyman et al., 1982). The more viscous a fluid is, the greater the shear stress needed to maintain a given velocity gradient. Dynamic viscosity is often expressed in terms of poise (gram per centimeter per second) or centipoise (0.01 poise). Water has a viscosity of approximately 1 centipoise at 20°C.

Viscosity varies with temperature, as indicated in Table 5-2, and with concentration of dissolved chemicals. The effect of pressure on fluid viscosity is generally unimportant (Mercer et al., 1982). Note that dynamic viscosity is a term in the relationship between hydraulic conductivity and intrinsic permeability (Section 5.1.4.2).

5.1.3.9 Time Integration Weighting Factor, W [--]

A value of W equal to 1.0 should be used for most practical problems (see Equation 3-16). Setting W equal to 0.5 is normally done for research purposes to assess the accuracy of the Crank-Nicolson scheme.

5.1.3.10 Relaxation Parameter for Solving the Nonlinear Equation, OME [--]

Normally this parameter should be set to 1.0 (see Equation 3-17). If the convergence history shows signs of oscillation, then a value of 0.5 should be used. If the convergence

TABLE 5-2. DYNAMIC VISCOSITY OF WATER AS A FUNCTION OF TEMPERATURE

Temperature (“c)	Dynamic Viscosity (centipoise)
o	1.7921
10	1.3077
20	1.0050
30	0.8007
40	0.6560
50	0.5494
100	0.2838

Source: CRC, 1965

history shows monotonic decreases but at a very slow rate, then OME should be set to somewhere between 1.7 to 1.9.

5.1.3.11 Iteration Parameter to Solve the Linearized Matrix Equation, OMI [--]

Normally this parameter should be set to 1.0 (see Equation 3-18). If the convergence history shows signs of oscillation, then set OMI to 0.5. If the solution converges monotonically but at a very slow rate, then set OMI to between 1.7 and 1.9.

5.1.4 Data Set 5: Material Properties

In the material properties data set, the user must input values for either hydraulic conductivity or permeability for each aquifer/soil material type. The flag that tells the code which of these two properties is being input is the permeability input control, KCP, located in Data Group 6.

5.1.4.1 The Saturated Hydraulic Conductivity Tensor [L/T]

Hydraulic conductivity is the coefficient of proportionality which appears in Darcy's Law. It expresses the ease with which a fluid can be transported through a porous medium and is a function of properties of both the porous medium and the fluid (Mills et al., 1985b). It is defined as the volume of water that will move in unit time under a unit hydraulic gradient through a unit area measured at right angles to the direction of flow. For three-dimensional flow in an anisotropic medium, hydraulic conductivity varies with direction at any point in space and is expressed as a symmetric second-rank tensor:

$$K_{ij} = \begin{bmatrix} K_{xx} & K_{xyy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zyy} & K_{zz} \end{bmatrix} \qquad (5\text{-}1)$$

where K_{ij} is the hydraulic conductivity tensor and x, y, and z are the coordinate axes of the model grid. Because of symmetry, only 6 of the 9 terms are needed (K_{xx}, K_{yy}, K_{zz}, and $K_{xy} = K_{yx}$, $K_{xz} = K_{zx}$, and $K_{yz} = K_{zy}$).

If the coordinate axes coincide with the principal directions of anisotropy, then the nine components of the tensor reduce to K_{xx}, K_{yy}, and K_{zz}, with the other components equal to zero. For isotropic media, hydraulic conductivity is independent of the direction of measurement (i.e., $K_{xx} = K_{yy} = K_{zz}$).

Hydraulic conductivity estimates should be based on site-specific data collection (e.g., pumping tests or piezometer tests). Some typical horizontal hydraulic conductivity values for various materials are shown in Table 5-3. Note that hydraulic conductivity varies over a very wide range. As a result, values are rarely known with more than an order-of-magnitude accuracy. Hydraulic conductivity values for fractured rock can be found in Mercer et al. (1982).

For many materials, the vertical hydraulic conductivity is substantially smaller than the horizontal hydraulic conductivity (assuming horizontal bedding and measurements made along the principal axes) (Mercer et al., 1982). Mills et al. (1985b) state that the ratio of horizontal to vertical conductivity, known as the anisotropy ratio, is from 2 to 10 for alluvium and glacial outwash and from 1.5 to 3 for sandstone. The variability in horizontal and vertical conductivities for a few aquifer materials is shown in Table 5-4.

5.1.4.2 The Permeability Tensor [L^2]

Intrinsic permeability is a property of the porous medium only. It is a measure of the resistance to fluid flow through the medium. The greater the permeability, the less the resistance. Like hydraulic conductivity, permeability is a symmetrical second-rank tensor. Permeability is equal to hydraulic conductivity multiplied by a scalar value, as is seen in the following equation:

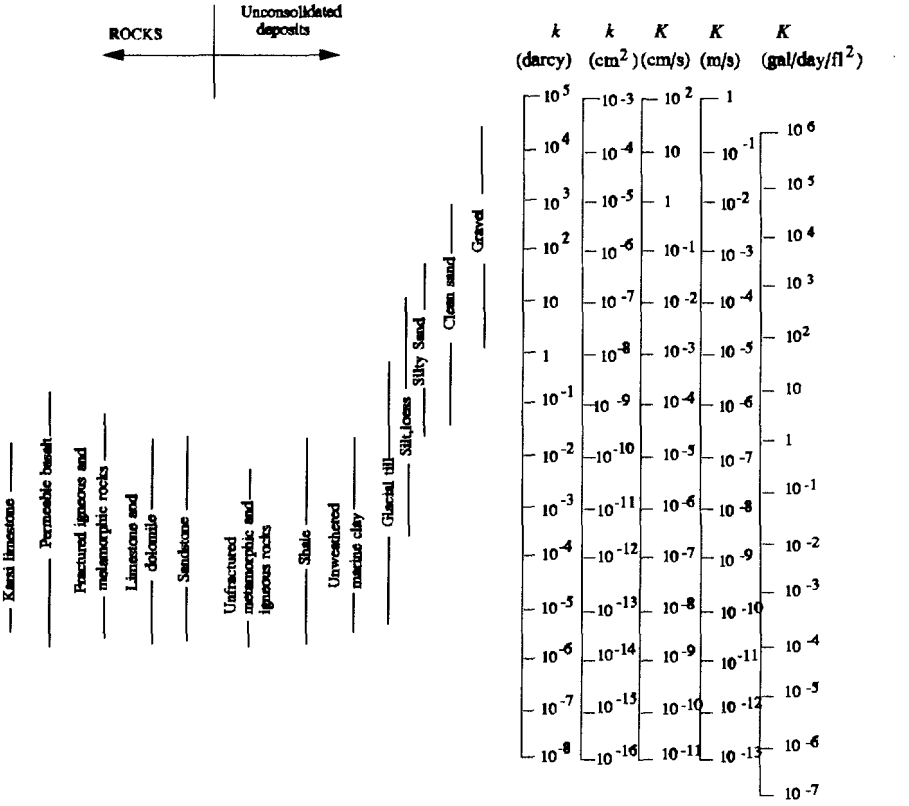
$$k_{ij} = K_{ij}\,\mu/(\rho g) \qquad (5\text{-}2)$$

where

k_{ij} = permeability (L')
K_{ij} = hydraulic conductivity (L/T)
μ = dynamic viscosity (M/L/T)
ρ = density (M/L^3)
g = acceleration of gravity (L/T^2)

As was true for hydraulic conductivity, permeability estimates should be based on site-specific data collection. Ranges of values for permeability are shown in Table 5-3 and in Table 5-5. Permeability is sometimes expressed in units of darcies. Conversion from darcies to other units can be done by using the conversion factors provided at the bottom of Table 5-3.

TABLE 5-3. RANGE OF HYDRAULIC CONDUCTIVITY VALUES FOR VARIOUS GEOLOGIC MATERIALS (Freeze and Cherry, 1979)



Conversion Factors for Permeability and Hydraulic Conductivity Units

	Permeability, k*			Hydraulic conductivity, K		
	cm^2	ft^2	darcy	m/s	ft/s	U.S. gal/day/ft^2
cm^2	1	$1.08x10^{-3}$	$1.01x10^{3}$	$9.80x10^{2}$	$3.22x10^{3}$	$1.85x10^{9}$
ft^2	$9.29x10^{2}$	1	$9.42x10^{10}$	$9.11x10^{5}$	$2.99x10^{6}$	$1.71x10^{12}$
darcy	$9.87X10^{-9}$	$1.06X10^{-11}$	1	$9.66X10^{-6}$	$3.17X10^{-5}$	$1.82X10^{1}$
m's	$1.02x10^{-3}$	$1.10x10^{-6}$	$1.04x10^{5}$	1	3.28	$2.12x10^{6}$
ft/s	$3.11x10^{-4}$	$3.35x10^{-7}$	$3.15x10^{4}$	$3.05x10^{-1}$	1	$6.46x10^{5}$
U.S. gal/ day/ft^2	$5.42x10^{-10}$	$5.83x10^{-13}$	$5.49x10^{-2}$	$4.72x10^{-7}$	$1.55x10^{-6}$	1

*To obtain k in ft^2, multiply k in cm^2 by 1.08×10^{-3}.

TABLE 5-4. VARIABILITY IN HORIZONTAL AND VERTICAL HYDRAULIC CONDUCTIVITIES

Rock Types	K_H, m/s	K_V, m/s	K_V/K_H
Shale	2.0×10^{-8}	1.0×10^{-8}	0.5
Siltstone-shale	2.1×10^{-6}	2.1×10^{-7}	0.1
Siltstone-shale	2.8×10^{-7}	3.0×10^{-8}	0.107
Sandstone	3.4×10^{-7}	3.4×10^{-7}	1.0

Source: Mercer et al., 1982; Original Reference: Golder Associates, 1977

TABLE 5-5. PERMEABILITY OF POROUS MATERIALS

Material		k (m^2)
Argillaceous limestone	2% porosity	9.87×10^{-17}
Limestone	16% porosity	1.38×10^{-13}
Sandstone, silty	12% porosity	2.57×10^{-15}
Sandstone, coarse	12% porosity	1.09×10^{-12}
Sandstone	29% porosity	2.37×10^{-12}
Very fine sand	well sorted	9.77×10^{-12}
Medium sand	very well sorted	2.57×10^{-10}
Coarse sand	very well sorted	3.06×10^{-9}
Gravel	very well sorted	4.24×10^{-8}
Montmorillonite clay[b]		10^{-17}
Kaolinite clay[b]		10^{-15}

[a] These are provided as estimates; actual values will vary.
[b] For the clays, only the order of magnitude is indicated.

Source: Mercer et al., 1982; Adapted from: Davis and DeWiest, 1966

5.1.5 Data Set 6: Soil Property Parameters

As was explained in Section 3.1.1, relationships between relative permeability and water content and between pressure head and water content must be specified in order to solve the governing equation for unsaturated flow. The 3DFEMWATER code provides two options for specifying these relationships. The user can 1) input parameters for analytical expressions of these relationships, or 2) input the coordinates of characteristic curves in tabular format. The analytical parameters are discussed first, followed by the tabular data requirements.

5.1.5.1 Analytical Parameters

Analytical equations developed by van Genuchten (1980) are used in the code to describe the relationship between pressure head and moisture content and the relationship between relative hydraulic conductivity and moisture content (see Equations 3-3a through 3-3d). In order to solve these equations, five parameters must be specified in the input sequence for each material type: residual moisture content, saturated moisture content, air entry pressure head, and two soil-specific empirical parameters, alpha and beta.

5.1.5.1.1 Residual and Saturated Moisture (Water) Content [--1

The volumetric moisture content, θ, is defined as:

$$\theta = V_W/V_T \tag{5-3}$$

where

VT = the total unit volume of a rock or soil (L^3)
VW = the volume of a rock or soil occupied by water (L^3)

The saturated moisture content is equal to the porosity of the medium since all of the void space is filled with fluid. Under unsaturated conditions, however, some of the void space is filled with air and thus, the moisture content is less than the medium's porosity. The residual moisture content is that amount which can not be removed from a soil by gravity drainage, even under large suction pressure, because it adheres to the grains of the soil.

Table 5-6 lists descriptive statistics for both saturated and residual moisture content for a variety of soil types. In addition, saturated and residual moisture content values for a large number of soils can be obtained using the interactive computer program DBAPE (Imhoff et al., 1990). DBAPE, which is a soils data base analyzer and parameter estimator, is available from the U.S. EPA Center for Exposure Assessment Modeling (CEAM) at the Environmental Research Laboratory in Athens, Georgia.

5.1.5.1.2 Air Entry Pressure Head [L]

The air entry pressure head is the threshold at which air starts to penetrate saturated soil. It is typically a very small negative value for fine-grained materials and zero for coarser materials. Its value can be estimated from the water retention curves of specific

TABLE 5-6. DESCRIPTIVE STATISTICS FOR SATURATION WATER CONTENT (θ_s) AND RESIDUAL WATER CONTENT (θ_r)

	Saturation Water Content (θ_s)				Residual Water Content (θ_r)			
	Statistic*							
Soil Type	$\bar{x}$	s	CV	n	x	s	CV	n
Clay**	0.38	0.09	24.1	400	0.068	0.034	49.9	353
Clay Loam	0.41	0.09	22.4	364	0.095	0.010	10.1	363
Loam	0.43	0.10	22.1	735	0.078	0.013	16.5	735
Loamy Sand	0.41	0.09	21.6	315	0.057	0.015	25.7	315
Silt	0.46	0.11	17.4	82	0.034	0.010	29.8	82
Silt Loam	0.45	0.08	18.7	1093	0.067	0.015	21.6	1093
Silty Clay	0.36	0.07	19.6	374	0.070	0.023	33.5	371
Silty Clay Loam	0.43	0.07	17.2	641	0.089	0.009	10.6	641
Sand	0.43	0.06	15.1	246	0.045	0.010	22.3	246
Sandy Clay	0.38	0.05	13.7	46	0.100	0.013	12.9	46
Sandy Clay Loam	0.39	0.07	17.5	214	0.100	0.006	6.0	214
Sandy Loam	0.41	0.09	21.0	1183	0.065	0.017	26.6	1183

* n = Sample size, $\bar{x}$ = Mean, s = standard deviation, CV = coefficient of variation (percent)

** Agricultural soil, less than 60 percent clay.

Source: Sharp-Hansen et al. (1990)
Original source Carsel and Parrish (1988)

soils (Freeze and Cherry, 1979; Sharp-Hansen et al., 1990). In practice, it is regularly assumed to be zero.

5.1.5.1.3 Van Genuchten Parameters, α [1/L]; β [--]

These are empirical parameters needed to solve the van Genuchten analytical equations which are used to model unsaturated flow (see Equations 3-3a through 3-3d). Descriptive statistics for these parameters have been reported by Carsel and Parrish (1988) for a variety of soils and are shown in Table 5-7.

5-7. DESCRIPTIVE STATISTICS FOR VAN GENUCHTEN WATER RETENTION MODEL PARAMETERS, α, ß, and γ (Carsel and Parrish 1988)

	Parameter α, cm^{-1}				Parameter ß				Parameter γ			
Soil Type	X	SD	CV	N	X	SD	CV	N	X	SD	CV	N
Clay[a]	0.008	0.012	160.3	400	1.09	0.09	7.9	400	0.08	0.07	82.7	400
Clay Loam	0.019	0.015	77.9	363	1.31	0.09	7.2	364	0.24	0.06	23.5	364
Loam	0.036	0.021	57.1	735	1.56	0.11	7.3	735	0.36	0.05	13.5	735
Loamy Sand	0.124	0.043	35.2	315	2.28	0.27	12.0	315	0.56	0.04	7.7	315
Silt	0.106	0.007	45.0	88	1.37	0.05	3.3	88	0.27	0.02	8.6	88
Silt Loam	0.020	0.012	64.7	1093	1.41	0.12	8.5	1093	0.29	0.06	19.9	1093
Silty Clay	0.005	0.005	113.6	126	1.09	0.06	5.0	374	0.09	0.05	57.1	374
Silty Clay Loam	0.010	0.006	61.5	641	1.23	0.06	5.0	641	0.19	0.04	21.5	641
Sand	0.145	0.029	20.3	246	2.68	0.29	20.3	246	0.62	0.04	6.3	246
Sandy Clay	0.027	0.017	61.7	46	1.23	0.10	7.9	46	0.18	0.06	34.7	46
Sandy Clay Loam	0.059	0.038	64.6	214	1.48	0.13	8.7	214	0.32	0.06	53.0	214
Sandy Loam	0.075	0.037	49.4	1183	1.89	0.17	9.2	1183	0.47	0.05	10.1	1183

X = Mean, SD = Standard Deviation, CV = Coefficient of Variation (percent), N = Sample Size

[a] = Agricultural Soil, Clay 60 percent

5.1.5.2 Tabular Data Parameters

If the user chooses to supply the soil moisture relationships in tabular form, four parameters must be specified for each functional data point: moisture content, the corresponding pressure head and relative permeability, and water capacity. Sets of these parameters must be input for each type of material being simulated. The necessary tabular data for a large number of soils can be obtained from the interactive computer code, DBAPE, described in Section 5.1.5.1.1, with the exception of water capacity.

Moisture content was described in Section 5.1.5.1.1. Pressure head, relative permeability, and water capacity are briefly introduced below.

5.1.5.2.1 Relative Permeability (or Hydraulic Conductivity) [--]

In an unsaturated porous medium, the permeability of the water phase in the medium is a function of the degree of saturation. The larger the degree of saturation, the larger the permeability associated with the water phase. This unsaturated permeability is also known as the effective permeability.

Relative permeability is defined as the ratio of the effective permeability to the permeability at saturation. Because it is a ratio, relative permeability ranges in value between 0.0 and 1.0. It is generally assumed that relative permeability is a scalar, dimensionless non-linear function, even for anisotropic soils. Because of the relation of equivalence, relative permeability is equal to relative hydraulic conductivity (Mercer et al., 1982).

Curves showing the relationship between relative permeability and moisture content are determined experimentally for individual soils. The tabulated data available in the literature or in DBAPE (Imhoff et al., 1990) are extracted from these experimental results.

5.1.5.2.2 Pressure head [L]

In groundwater hydrology, the total hydraulic head, H, is usually considered to be the sum of two components: elevation head, z, and pressure head, h. The contribution of velocity to the total head is neglected because velocities are usually extremely low. Pressure head is measured in gage pressure. In the saturated zone, pressures are greater than atmospheric and are thus recorded as positive pressures. The water table is defined as the location at which pressure is equal to atmospheric. This implies that pressure head is zero and the total head is equal to the elevation head. Above the water table, pressure head is less than atmospheric and water is held in the pore spaces under tension or suction. Thus, pressure head values in the unsaturated zone are negative.

Pressure head in the unsaturated zone is a function of moisture content--the lower the moisture content, the more negative the pressure head. As moisture content increases, the surface tension forces holding the water in place between the grains of soil are lowered, resulting in less negative pressure heads (Freeze and Cherry, 1979). The characteristic curve showing the relationship between pressure head and moisture content is determined experimentally for each porous medium.

5.1.5.2.3 Moisture Content Capacity [l/L]

In an unsaturated soil, changes in moisture content, 9, are accompanied by changes in pressure head, h. As discussed above, the 6(h) relationship results in a characteristic curve for each soil. Example characteristic curves are shown in Figure 3.3a. The inverse of the slope of this curve is called the water capacity, $C(\theta)$, or the moisture content capacity (Mercer et al., 1982). It is defined as:

$$C(\theta) = d\theta/dh \qquad (5\text{-}4)$$

The water capacity has no one unique value for a porous medium. Thus, the range of values of moisture content capacity is related to the nature of the water characteristic curve. (Mercer et al., 1982).

5.2 3DLEWASTE

5.2.1 Data Set 1: Title of the Simulation Run

5.2.1.1 Geometry, Boundary, and Pointer Array Control, IGEOM [--]

The integer IGEOM has two functions. It is used to specify if geometry, boundary, and pointer arrays should be printed so that the user can examine them. It also controls whether the boundary and pointer arrays are written to or read from binary files. Boundary arrays store data related to the boundary conditions. Pointer arrays store the global matrix in compressed form and are used to construct the subregional block matrices. For large problems, it takes too much time to generate these arrays for each computer execution of a particular scenario.

If 3DLEWASTE is being executed alone (i.e., without using 3DFEMWATER results), these arrays should be generated only once and stored in binary files using logical units LUBAR and LUPAR (see Table B-2). In order to compute and store the boundary and pointer arrays, the user should choose a value for IGEOM less than or equal to one. In subsequent runs, the boundary and pointer arrays can be read from the binary files by changing the value of IGEOM to a number greater than three. Whenever changes are made to the model which involve the geometry of the problem, the boundary conditions, and the configuration of the subregions, the arrays must be generated and stored again.

If 3DLEWASTE is run after executing 3DFEMWATER for the same scenario, the boundary array need not be recalculated (i.e., the boundary array calculated and stored by 3DFEMWATER can be used). The pointer array should be recalculated, however. This is done by setting IGEOM to a value greater than one and less than or equal to three.

For each of the options explained above, if the number chosen by the user is even, the arrays will be printed as output. If the number is odd, the arrays will not be printed.

5.2.2 Data Set 2: Basic Integer Parameters

5.2.2.1 Number of Material Types, NMAT [--]

This parameter is the total number of different material types being modeled. When material properties are assigned to each material type, using data set 5 (see Section 4.2.5), the first material type should be the predominant type. The number of material types used in 3DLEWASTE need not be identical to the number specified in 3DFEMWATER.

5.2.2.2 Number of Elements with Material Property Correction, NCM [--]

In the code, all the grid elements automatically are initialized as having a material type of one. To model more than one material type, the parameter NCM and the parameters in data set 9 of the input (see Section 4.2.9) are used to specify which elements have a material type other than material type one. The parameter NCM is the total number of elements which have a material type different than the first material type.

5.2.2.3 Number of Time-Steps, NTI [--]

For a constant time-step size, this number is obtained by dividing the simulation time by the time-step size, DELT. If the time-step size is variable, this number is computed using the formula given in the note at the end of data set 2 in Section 4.2.2.

5.2.2.4 Steady-State Control, KSS [--]

As noted in Section 4.2.2, a steady-state option may be used to provide either the final state of a system under study or the initial condition for a transient-state calculation. In the former case, both KSS and the number of time steps, NTI, should be set to zero. In the latter case (i.e., when KSS = 0 and NTI > 0), the code performs a steady-state calculation before beginning the transient computations. If KSS = 1, no steady-state calculation is performed. Rather, the code begins transient calculations using initial conditions supplied in data set 10 of the input.

5.2.2.5 Mass Lumping Flag, ILUMP [--]

This parameter indicates if the mass matrix is to be lumped or not. Normally, one should set this parameter to 0. Without lumping, the solution is more accurate. However, for occasions when negative concentrations or oscillating solutions occur, this parameter should be set to 1.

5.2.2.6 Weighting Function Control, IWET [--]

This parameter indicates if the upstream weighting function is to be used. For the present version of code, this parameter does not affect the solution when a transient solution is sought. If a steady-state solution is desired, one should set this parameter to 1. Thus, it is advisable to always set this parameter to 1 for the present version of the computer code.

5.2.2.7 Optimization Flag, IOPIYM [--]

This parameter specifies whether the upstream weighting factor is to be optimized. This parameter does not affect the solution if a transient solution is sought. For a steady-state solution, it is advisable to set IOPTIM to 1. When IOPTIM is set to O, an upstream weighting factor of 1.0 is assumed.

5.2.2.8 Number of Iterations for the Nonlinear Equation, NITER [--]

This parameter is the number of iterations allowed for solving the nonlinear equation. Normally, a value of NITER equal to 40 should be sufficient. If this number is exceeded and the solution does not converge, the program will issue a warning message. When this occurs, the users should re-execute the program using a larger value of NITER.

5.2.2.9 Number of Times to Reset the Time Step, NDTCHG [--]

This parameter indicates how many times one should reset the time step size to the initially small time-step size. When we start a computation, we normally use a small time-step size. However, for every consecutive time step, we may gradually increase the time-step size by some amount specified by CHNG in Data Set 3 in Section 4.2.3. When we have a steep change in boundary conditions or in source/sink conditions, we will need to reset the time-step size to the initially small value. NDTCHG tells us how many times we want to reset the time-step size. The value of NDTCHG must be at least one. If the user does not want to reset the time step, a value of one should be entered here and a very large number, larger than the total simulation time, should be entered for TDTCH(l) in data set 4 (see Section 4.2.4).

5.2.2.10 Number of Iterations for Pointwise Solution, NPITER [--]

This parameter is used to input the number of iterations allowed for solving the matrix equations with the block iteration method. NPITER = 300 should be sufficient for most problems. If this number is exceeded and the solution does not converge, the program will issue a warning message. When this occurs, the user should first recheck the input values. If the input is correct, the program can be re-executed using a larger value for NPITER.

5.2.2.11 Sorption Model Control, KSORP [--]

Although the Freundlich isotherm option can be used to simulate a linear isotherm by setting the value of the exponent, n, equal to one, it is recommended that linear isotherms be simulated using only the linear isotherm option. This is because the linear isotherm option makes use of retarded seepage velocities, which result in a more accurate solution for the particle tracking scheme used in 3DLEWASTE than the pore velocities used in conjunction with the nonlinear adsorption models.

5.2.3 Data Set 3: Basic Real Parameters

5.2.3.1 Initial Time-Step Size, DELT [T]

This is the time-step size used for the first time-step computation if the variable CHNG is not equal 0.0. It is the time-step size used for every time step if the variable CHNG is set equal to 0.0. For a steady-state computation, DELT should be chosen such that no particle travels more than one element in one time step. For example, if an element has a size of 10 m and the averaged velocity over this element is 0.00001 m/see, then DELT should be less then 1,000,000 seconds. For transient computations, one should choose a time-step size as large as possible with DELT less than DELX*DELWD, where DELX is the size of the element and D is the dispersion coefficient. For example, if the element size is 10 m and the dispersion coefficient is 0.00001 m^2/sec, then DELT should be less than 10,000,000 seconds.

5.2.3.2 Fractional Change in Time-Step Size, CHNG [--]

This parameter specifies how much of an increase one would like to make to the time-step size for each subsequent time step. Normally, a value from 0.0 to 0.5 can be used.

5.2.3.3 Maximum Allowable Time Step, DELMAX [T]

The maximum time-step size allowed depends on how fast the system responds to change. Use of a value one to ten times the size of the initial time step is advised.

5.2.3.4 Maximum Simulation Time, TMAX [T]

This is the actual length of time to be simulated. If this time is exceeded before you have made NTI step computations, the simulation will be terminated.

5.2.3.5 Relaxation Parameter for Solving the Nonlinear Equation, OME [--]

Normally this parameter should be set to 1.0 (see Equation 3-48). If the convergence history shows sign of oscillation, then a value of 0.5 should be used. If the convergence history shows monotonic decreases but at a very slow rate, then OME should be set to somewhere between 1.7 to 1.9.

5.2.3.6 Iteration Parameter to Solve the Linearized Matrix Equation, OMI [--]

Normally this parameter should be set to 1.0 (see Equation 3-49). If the convergence history shows signs of oscillation, then set OMI to 0.5. If the solution converges monotonically but at a very slow rate, then set OMI to between 1.7 and 1.9.

5.2.3.7 Transient Convergence Criterion, TOLB [--]

This is the relative error allowed for assessing if a solution has converged for each time step. Setting TOLB equal to 0.000001 should be sufficient for most problems.

5.2.3.8 Steady-State Convergence Criterion, TOLA [--]

This is the relative error allowed for assessing if a steady-state solution has converged. TOLA = 0.00001 should be sufficient for most problems.

5.2.4 Data Set 5: Material Properties

5.2.4.1 Distribution Coefficient [L^3/M]

Freeze and Cherry (1979) state that adsorption/desorption reactions for contaminants in groundwater are normally viewed as being very rapid relative to the flow velocity and that the amount of contaminant adsorbed is commonly a function of concentration in the solution. At constant temperature and low-to-moderate concentrations, the functional relationship between the adsorbed concentration, S (M/L^3), and the dissolved concentration, C (M/L^3), is often approximated by the Freundlich equilibrium isotherm (Helfferich, 1962):

$$S = KC^n \tag{5-5}$$

where the coefficients K and n depend on several factors, including the solute species and the nature of the porous medium. If the isotherm is linear, n = 1, K is known as the distribution coefficient, K_d. The derivation of the distribution coefficient, which is different for each constituent, is discussed briefly in Section 3.3.1.

5.2.4.2 Bulk Density [M/L^3]

Bulk density can be defined as the mass of a unit volume of dry soil. The soil bulk density directly influences the retardation of solutes and is related to the structure and texture of a soil (Mercer et al., 1982).

The bulk density of soils typically range between 1.3 and 2.0 g/cm^3, but Mercer et al. (1982) state that the bulk density can be as low as 0.3 g/cm^3 for soils high in organics or aluminum and iron hydroxides. Representative values for five different types of soils are shown in Table 5-8. In addition, values of bulk density for a large number of soils can be obtained from the interactive computer program DBAPE, which was discussed in Section 5.1.5.1.1.

The bulk density of aquifer materials may differ significantly from that of soils. Therefore, data on the ranges of bulk density for various geologic material are presented in Table 5-9. If site-specific data are not available, the bulk density of the saturated zone can be derived using an exact relationship between porosity, particle density and the bulk density (Freeze and Cherry, 1979). Assuming the particle density to be 2.65 g/cm^3, we can express this relationship as:

$$\rho_b = 2.65(1 - \theta) \tag{5-6}$$

where

ρ_b = bulk density of the soil (g/cm^3)
θ = saturated moisture content (porosity) (--)

TABLE 5-8. MEAN BULK DENSITY (g/cm^3) FOR FIVE SOIL TEXTURAL CLASSIFICATIONS[a,b]

Soil Texture	Mean Value	Range Reported
Silt Loams	1.32	0.86-1.67
Clay and Clay Loams	1.30	0.94-1.54
Sandy Loams	1.49	1.25-1.76
Gravelly Silt Loams	1.22	1.02-1.58
Loams	1.42	1.16-1.58
All Soils	1.35	0.86-1.76

[a] Baes, C. F., III and R.D. Sharp. 1983. A Proposal for Estimation of Soil Leaching Constants for Use in Assessment Models. J. Environ. Qual. 12(1):17-28 (Original reference).

[b] From Dean et al. (1989)

5.2.4.3 Longitudinal and Transverse Dispersivity [L]

Hydrodynamic dispersion is a non-steady, irreversible mixing process by which a contaminant spreads as it is transported through the subsurface. It results from the effects of two components: molecular diffusion and mechanical dispersion. The larger the hydrodynamic dispersion term is, the larger the spreading of an initially localized contaminant. Molecular diffusion is discussed in Section 5.2.4.4. Mechanical dispersion, **D,** is caused by variations in pore velocities in a soil or aquifer material. In addition, variations in the rate of advection caused by aquifer inhomogeneity and spatially-variable hydraulic conductivities results in plume spreading, which is often confused with dispersion (Keely, 1989).

Although mechanical dispersion is a second rank tensor, by assuming that a material is isotropic with respect to dispersion, the dispersion tensor can be expressed in terms of the average groundwater velocity and two constants: the longitudinal and transverse dispersivity (see Equation 3-20). Longitudinal dispersivity, α_L, is defined as the characteristic mixing length in the direction of groundwater flow and lateral dispersivity, α_T, is the mixing length in the directions perpendicular to flow.

Values for dispersivity are difficult to determine. Research has shown that the values are dependent on the scale of the problem being studied (EPRI, 1985). This can be seen in Figure 5.1. Usually, dispersion is determined by adjusting the dispersivity values until modeling results match historical data (Mercer et al., 1982). Transverse dispersivity values are commonly thought to be lower than longitudinal dispersivity values by a factor of 3 to 20. However, recent studies suggest that transverse dispersivity values should be at least an order-of-magnitude smaller than longitudinal dispersivity values (Gelhar et al., 1992) and may even be close to zero (U.S. EPA, 1989).

TABLE 5-9. RANGE AND MEAN VALUES OF DRY BULK DENSITY FOR VARIOUS GEOLOGIC MATERIALS

Material	Range (g/cm^3)	Mean (g/cm^3)
Clay	1.18-1.72	1.49
Silt	1.01-1.79	1.38
Sand, fine	1.13-1.99	1.55
Sand, medium	1.27-1.93	1.69
Sand, coarse	1.42-1.94	1.73
Gravel, fine	1.60-1.99	1.76
Gravel, medium	1.47-2.09	1.85
Gravel, coarse	1.69-2.08	1.93
Loess	1.25-1.62	1.45
Eolian sand	1.33-1.70	1.58
Till, predominantly silt	1.61-1.91	1.78
Till, predominantly sand	1.69-2.12	1.88
Till, predominantly gravel	1.72-2.12	1.91
Glacial drift, predominantly silt	1.11-1.66	1.38
Glacial drift, predominantly sand	1.36-1.83	1.55
Glacial drift, predominantly gravel	1.47-1.78	1.60
Sandstone, fine grained	1.34-2.32	1.76
Sandstone, medium grained	1.50-1.86	1.68
Siltstone	1.35-2.12	1.61
Claystone	1.37-1.60	1.51
Shale	2.20-2.72	2.53
Limestone	1.21-2.69	1.94
Dolomite	1.83-2.20	2.02
Granite, weathered	1.21-1.78	1.50
Gabbro, weathered	1.67-1.77	1.73
Basalt	1.99-2.89	2.53
Schist	1.42-2.69	1.76

Reference: Morris and Johnson (1967); Mills et al. (1985b)

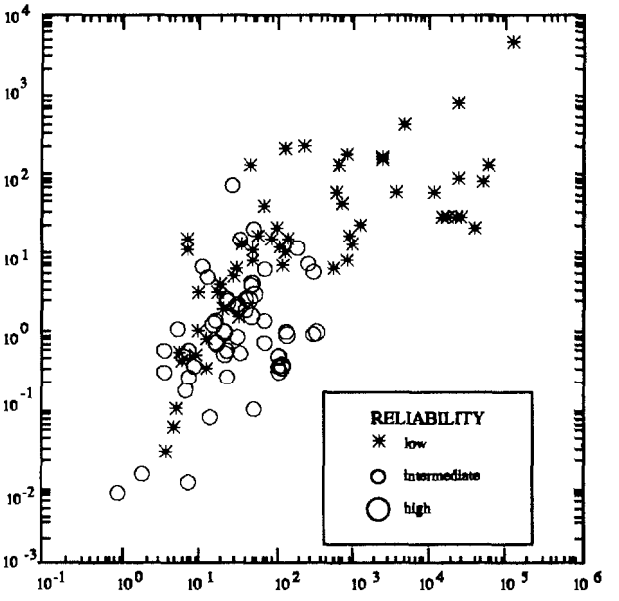


Figure 5.1. Longitudinal dispersivity versus scale with data classified by reliability (from Gelhar et al., 1992).

As initial estimates for longitudinal and transverse dispersivity, Dean et al. (19$9) suggest the following relationships, based on values presented in the Federal Register (1986):

$$\alpha_L = 0.1\ x_r \tag{5-7a}$$

$$\alpha_T = \alpha_L/3.0 \tag{5-7b}$$

where x_r is the distance from the source to a downgradient point of interest.

5.2.4.4 Molecular Diffusion Coefficient in Water $[L^2/T]$

As stated above, molecular diffusion and mechanical dispersion are both responsible for the dispersion of solutes in groundwater systems. Molecular diffusion, which is a non-reversible process, is typically small compared to mechanical dispersion and is often neglected in groundwater studies. However, when groundwater velocities are very low, molecular diffusion can become significant.

The flux of a solute in a fluid due to molecular diffusion is described by Fick's Law, which states that the flux is proportional to the concentration gradient. The coefficient of proportionality is called the molecular diffusion coefficient, a_m. Values for the molecular diffusion coefficient in a fluid continuum are generally well known and are

typically in the range of 10^{-9} m^2/s or less at 20°C. If necessary, a_m, which varies with temperature, can be estimated from methods described in Lyman et al. (1982).

5.2.4.5 Tortuosity [--]

The molecular diffusion coefficient for a solute in a porous medium is smaller than the coefficient of diffusion in a body of water because diffusion in solids is negligible. The amount by which the molecular diffusion coefficient is reduced is expressed by a coefficient called tortuosity. Tortuosity is a second-rank tensor which for isotropic conditions reduces to a scalar. It expresses the effect of the configuration of the water occupying a porous medium (Bear and Verruijt, 1987).

De Marsily (1986) states that a medium's tortuosity, τ, can be defined as:

$$\tau = 1/F\phi \tag{5-8}$$

where

F = formation factor (the ratio of a rock's electric resistivity over the resistivity of its contained water) (--)
ϕ = total porosity (--)

The author states that tortuosity varies in practice from 0.1 for clays to 0.7 for sands. Freeze and Cherry (1979) state that the coefficient, which is always less than one, usually has a value between 0.01 and 0.5.

Bresler (1973), as found in Dean et al. (1989), provides the following equation to estimate diffusion coefficient in a porous medium:

$$D_m = D_w\, ae^{b\theta} \tag{5-9}$$

where

D_m = coefficient of diffusion in a porous medium (cm^2/day)
D_w = coefficient of diffusion in water (cm^2/day)
a = soil constant having a range of 0.001 to 0.005
b = soil constant having an approximate value of 10
θ = volumetric water content (cm^3/cm^3)

In the above equation, the term $ae^{b\theta}$ represents an estimate of the soil's tortuosity.

5.2.4.6 Decay Constant [1/T]

A number of processes, such as hydrolysis and biodegradation, contribute to the disappearance of chemicals in the subsurface. The extent to which these processes are important depends on both environmental conditions and the chemical's properties. In this model, the effects of individual processes on the degradation of a chemical in the subsurface are not considered. Instead, lumped first-order decay with respect to the concentration of the solute is assumed to occur, with a single first-order decay constant controlling the modelled rate of disappearance in each porous material.

When estimating a value for the first-order decay constant, one should determine which processes are likely to be important at the study area. Hydrolysis is a potentially significant elimination pathway for many organic chemicals. However, for chemicals that readily biodegrade, hydrolysis may be insignificant relative to biodegradation. Methods of estimating a first-order rate constant resulting from hydrolysis are presented in Lyman et al. (1982). Values for hydrolysis rate constants can be found in a large number of references, including Lyman et al. (1982), Mabey et al. (1982), and Mills et al. (1985a).

Although biodegradation is the most significant means of removal for many organics in the subsurface, it is a very complex and poorly understood process. Biodegradation in the subsurface depends on a number of variable and/or unknown processes, such as the number of microorganisms present, the availability of oxygen and other nutrients, and the Ph and temperature of the subsurface environment (Sharp-Hansen et al., 1990). Therefore it is very difficult to estimate the first-order decay coefficient resulting from biodegradation. Laboratory-derived biodegradation rate constants have been compiled by Lyman et al. (1982), Mabey et al. (1982), and Mills et al. (1985a), among others. However, these laboratory-based values may be inappropriate for field conditions. Therefore, considerable care should be exercised if these data are used.

5.2.5 Data Set 17: Hydrological Variables

For most wellhead protection applications of this code, the velocity field and moisture content field will not need to be specified in the input. Instead, these variables should be calculated and stored by the variably-saturated flow code, 3DFEMWATER. The stored arrays of data are then accessed by 3DLEWASTE. Only when 3DLEWASTE is executed without first running 3DFEMWATER does the user need to supply values for these variables. Moisture content was introduced in Section 5.1.5.1.1 and will not be discussed here.

5.2.5.1 Velocity Field [L/T]

The velocity distribution is needed to quantify transport by advection. Groundwater velocities are routinely determined indirectly using measurements of hydraulic head, hydraulic conductivity, and Darcy's equation. For the case when the x, y, and z axes coincide with the principal directions of anisotropy, Darcy's Law, in terms of the Darcy velocity, is written as:

$$v_x = -K_x \, dh/dx \qquad (5\text{-}10a)$$

$$v_y = -K_y \, dh/dy \qquad (5\text{-}10b)$$

$$v_z = -K_z \, dh/dz \qquad (5\text{-}10c)$$

where K_x, K_y, and K_z are the hydraulic conductivity values in the x, y, and z directions, and dh/dx, dh/dy, and dh/dz are the hydraulic gradients in the x, y, and z directions. A more generalized form can be written as:

$$v_x = -K_{xx}\, dh/dx - K_{xy}\, dh/dy - K_{xz}\, dh/dz \qquad (5\text{-}ha)$$

$$v_y = -K_{yx}\, dh/dx - K_{yy}\, dh/dy - K_{yz}\, dh/dz \qquad (5\text{-}llb)$$

$$v_z = -K_{zx}\, dh/dx - K_{zy}\, dh/dy - K_{zz}\, dh/dz \qquad (5\text{-}llc)$$

Since velocity depends on the gradient as well as the hydraulic conductivity, its range is somewhat arbitrary. A range of velocities is given in Figure 5.2.

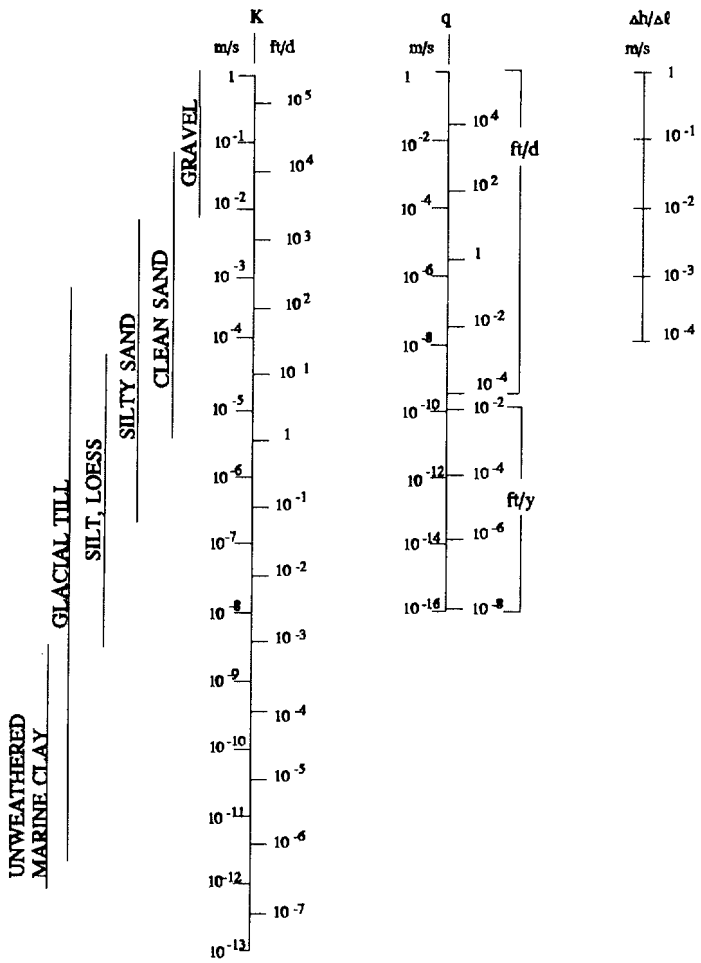


Figure 5.2. Nomograph for determining Darcy velocity (from Mercer et al., 1982)

SECTION 6

EXAMPLE PROBLEMS

6.1 3DFEMWATER

To demonstrate the application of 3DFEMWATER, three simple example problems are presented. These three problems represent one-, two-, and three-dimensional applications, respectively. For each problem, a brief description and a correctly-constructed input data set are given. The corresponding output is not included in this documentation. Rather, it is distributed along with the code by the EPA Center for Exposure Assessment Modeling (CEAM) at the Environmental Research Laboratory in Athens, Georgia. See Section 2 for information about obtaining the code.

6.1.1 One-Dimensional Column

One-dimensional transient flow through a column is simulated in this example. The column is 200 cm long and is 50 cm by 50 cm in cross-section (Figure 6.1). The soil in the column is assumed to be a sandy clay loam which has a saturated hydraulic conductivity of 31.4 cm/d, a porosity of 0.39 and a residual moisture content of 0.10. The unsaturated characteristic hydraulic properties of the soil in the column are represented by the van Genuchten analytical functions with the empirical coefficient alpha equal to 0.059 and the empirical coefficient beta equal to 1.48.

The initial conditions assumed are a pressure head of -90.0 cm imposed on the top surface of the column, 0.0 cm on the bottom surface of the column, and -97.0 cm elsewhere. The boundary conditions are as follows. No flux is imposed on the left, front, right, and back surfaces of the column (this is done automatically by the code). Pressure head is held at 0.0 cm on the bottom surface using a Dirichlet boundary condition. A variable boundary condition is used on the top surface of the column with a pending depth of zero, minimum pressure of -90.0 cm, a rainfall of 5.0 cm/d for the first 10 days, and a potential evaporation of 5.0 cm/d for the second 10 days.

The region of interest, that is, the whole column, is discretized with 1 x 1 x 40 = 40 elements with the element size equal to 50 x 50 x 5 cm. This results in 2 x 2 x 41 = 164 node points. For this simulation, each of the four vertical lines is considered a subregion. Thus, a total of four subregions, each with 41 node points, is used for the subregional block iteration simulation.

A variable time step size is used. The initial time step size is 0.05 days, and each subsequent time step size is increased by 0.2 times with a maximum time step

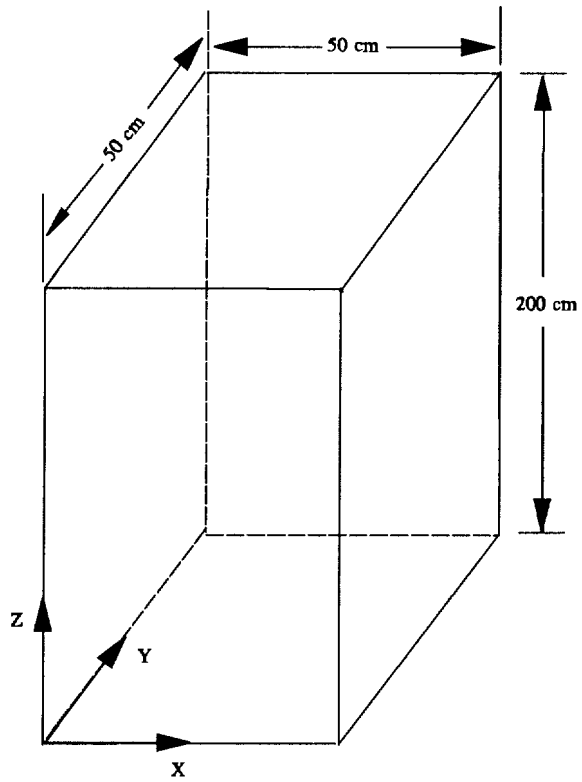


Figure 6.1. One-dimensional transient flow through a soil column.

size not greater than 1.0 d. Because there is an abrupt change in the flux value from 5 cm/d (infiltration) to -5 cm/d (evaporation) imposed on the top surface at day 10, the time step size is automatically reset to 0.05 d on the tenth day. Because a 20-day simulation is to be made, 44 time steps are needed.

A pressure head tolerance of 0.02 cm is selected for the nonlinear iteration and a tolerance of 0.01 cm is used for the block iteration. The relaxation factors for both the nonlinear iteration and block iteration are set equal to 0.5.

The input data set for this problem, prepared according to the instructions in Sections 4.1 and 5.1, is shown in Table 6-1.

6.1.2 Two-dimensional Drainage Problem

Two-dimensional steady-state flow is simulated in this problem. The region of interest is bounded on the left and right by parallel drains which fully penetrate the medium. The bottom is an impervious layer and the top is an air-soil interface (Figure 6.2). The distance between the two drains is 20 m. The medium is assumed to have a saturated horizontal hydraulic conductivity of 0.31 m/d and vertical hydraulic conductivity of 0.12 m/d, a porosity of 0.39, and a field capacity of 0.10. The unsaturated characteristic

TABLE 6-1. INPUT DATA SET FOR THE ONE-DIMENSIONAL 3DFEMWATER PROBLEM

```
   1 SIMULATION OF ONE-D COLUMN INFILTRATION-EVAPORATION; L=CM, T=DAY, M=G 011
C ******* DATA SET 2: BASIC INTEGERS
   164     40      1       0       44      1       6       1       0       0       50      20      3       100
C ******* DATA SET 3: BASIC REAL PARAMETERS
    0.05D0     0.2D0     1.0D0     20.0D0     2.0D-2     2.0D-2     1.0D0     7.316D12
   1.1232D2     1.0D0     0.5D0     0.5D0
C ******* DATA SET 4: PRINTER, STORAGE CONTROL AND TIME STEP SIZE RESETTING
33303030003000300300003330303000300030030003
11101010001000100100001110101000100010010001
   1.0D01       2.0000D1   1.0D38
C ******* DATA SET 5: MATERIAL PROPERTIES
    0.0D0       0.0D0     31.40D0       0.0D0       0.0D0       0.0D0
C ******* DATA SET 6: SOIL PROPERTY PARAMETERS
   0      5      0
  0.100D0       0.390D0       0.00D0       0.059D0       1.48D0                THPROP
C ******* DATA SET 7: NODE COORDINATES
    1     40     1          0.0D0          50.0D0       0.0D0       0.0D0       0.0D0       5.0D0
   42     40     1          0.0D0           0.0D0       0.0D0       0.0D0       0.0D0       5.0D0
   83     40     1          50.0D0          0.0D0       0.0D0       0.0D0       0.0D0       5.0D0
  124     40     1          50.0D0          50.0D0      0.0D0       0.0D0       0.0D0       5.0D0
    0      0     0          0.0             0.0         0.0         0.0         0.0         0.0
C ******* DATA SET 8: SUBREGIONAL DATA
    4
    1     3     1     41     0
    0     0     0     0      0                                  END OF NNPLR(K)
    1    40     1     1      1
    0     0     0     0      0                                  END OF GNLR(I,1)
    1    40     1     42     1
    0     0     0     0      0                                  END OF GNLR(I,2)
    1    40     1     83     1
    0     0     0     0      0                                  END OF GNLR(I,3)
    1    40     1     124    1
    0     0     0     0      0                                  END OF GNLR(I,4)
C ******* DATA SET 9: ELEMENT INCIDENCES
    1    39     1     42     83     124     1     43     84     125     2     1
    0     0     0     0      0       0      0      0      0      0      0     0                  END OF IE
C ******* DATA SET 11: INITIAL CONDITIONS
      1     3     41          0.0D0       0.0D0       0.0D0
      2    38     1          -9.70D1     0.0D0       0.0D0
     43    38     1          -9.70D1     0.0D0       0.0D0
     84    38     1          -9.70D1     0.0D0       0.0D0
    125    38     1          -9.70D1     0.0D0       0.0D0
     41     3     41         -9.00D1     0.0D0       0.0D0
      0     0     0          0.0         0.0         0.0                END OF IC
C ******* DATA SET 12: SOURCE/SINK AND B. C. CONTROL INTEGERS
    0      0      0      0      0      0      0      0      4      1      2      0
    1      4      1      4      0      0      0      0      0      0      0      0      0      0      0
```

TABLE 6-1. INPUT DATA SET FOR THE ONE-DIMENSIONAL 3DFEMWATER PROBLEM (concluded)

```
C ******* DATA SET 14: VARIABLE BOUNDARY CONDITIONS
    0.0D0       5.0D0       10.0D0      5.0D0       10.001D0    -5.0D0      1.0D38      -5.0D0
    1     0     0     1     0
    0     0     0     0     0           END OF IRTYP
    1     0     0     82    123   164   41    0     0     0     0
    0     0     0     0     0     0     0     0     0     0     0     END OF ISV(J,I) J=1,4
    1     3     1     41    41
    0     0     0     0     0                 END OF NPVB
    1     3     1           0.0D0       0.0D0       0.0
    0     0     0           0.0         0.0         0.0         END OF HCON
    1     3     1           -90.0D0     0.0D0       0.0
    0     0     0     0.0   0.0         0.0                     END OF HMIN
C ******* DATA SET 15: DIRICHLET BOUNDARY CONDITIONS
    0.0D0       0.0D0       1.0D38      0.0D0
    1     42    83    124
    1     3     1     1     0
    0     0     0     0     0                       END OF IDTYP
    0                 END OF JOB ----------------------------------------------------------------------------000
```

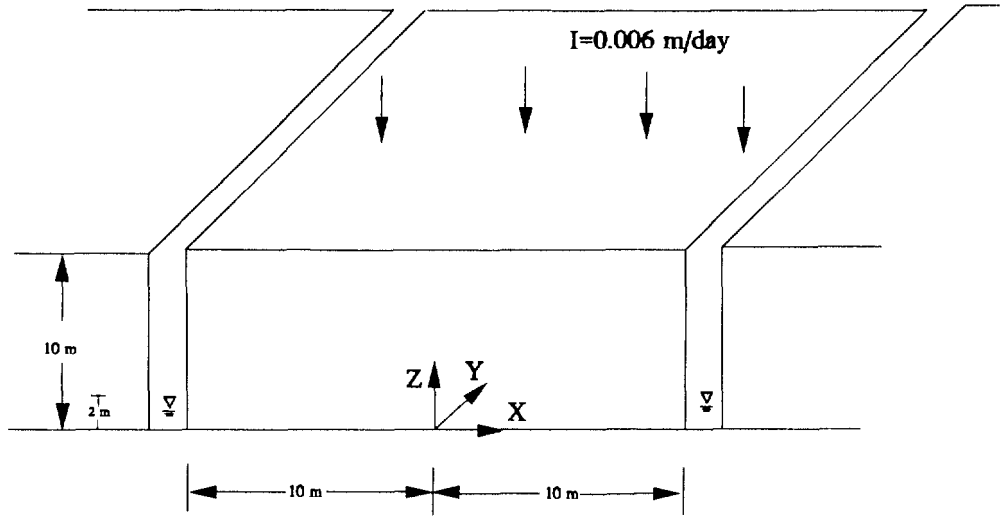


Figure 6.2. Two-dimensional steady-state flow to parallel drains.

hydraulic properties of the medium are given by the van Genuchten analytical functions with the empirical coefficient alpha equal to 0.059 and the empirical coefficient beta equal to 1.48.

Because of symmetry, the region to be simulated is $0.0 < x < 10.0$ m and $0.0 < z < 10.0$ m, with a width of 10 m assumed in the y-direction. A no flux boundary is imposed on the left ($x = 0.0$), front ($y = 0.0$), back ($y = 10.0$), and bottom ($z = 0.0$) sides of the region. Pressure head is assumed to vary from zero at the water surface ($z = 2.0$) to 2.0 m at the bottom ($z = 0.0$) on the right side ($x = 10.0$). Variable conditions are used elsewhere. Pending depth is assumed to be zero meters on the whole variable boundary. Fluxes on the top of the variable boundary are assumed equal to 0.006 m/d and on the right side, above the water surface, are equal to zero. A pre-initial condition for the steady-state solution is set as $h = 10 - z$.

The region of interest is discretized with 10 x 1 x 10 = 100 elements with the element size equal to 1 x 10 x 1 cm. This results in 11 x 2 x 11 = 242 nodal points. Each of the two vertical planes is considered a subregion. Thus, a total of two subregions, each with 121 node points, is used for the subregional block iteration simulation.

A pressure head tolerance of 0.002 m is set for the for nonlinear iteration and a value of 0.001 m is used for the block iteration. The relaxation factors for both the nonlinear iteration and block iteration are set equal to 0.5.

The input data set for this problem, prepared according to the instructions in Sections 4.1 and 5.1, is shown in Table 6-2.

6.1.3 Three-Dimensional Pumping Problem

Three-dimensional steady-state flow to a pumping well is simulated in this problem. The region of interest is bounded on the left and right by hydraulically connected rivers; on the front, back, and bottom by impervious confining beds; and on the top by an air-soil interface (Figure 6.3). A pumping well is located at (x,y) = (540,400) in Figure 6.3. Initially, the water table is assumed to be horizontal and is 60 m above the bottom of the aquifer. The water level at the well is then lowered to a height of 30 m. This height is held until a steady state condition is reached. The medium in the region is assumed to be anisotropic and has saturated hydraulic conductivity components K_{xx} = 0.31 m/d, K_{yy} = 0.03 m/d, and K_{zz} = 0.12 m/d. The porosity of the medium is 0.10 and the field capacity is 0.39. The unsaturated characteristic hydraulic properties of the medium are given by the van Genuchten analytical functions with the empirical coefficient alpha equal to 0.059 and the empirical coefficient beta equal to 1.48.

Because of symmetry, the region to be simulated is taken as $0 < x < 1000$ m, $0 < y < 400$ m, and $0 < z < 72$ m. Two types of boundary conditions are used. Pressure head is assumed hydrostatic on two vertical planes. The first is located at $x = 0$ and $0 < z < 60$ and the second, at $x = 1000$ and $0 < z < 60$. A no flux boundary is imposed on all other boundaries of the flow regime. The pre-initial condition for the steady-state solution is set so that the pressure head, $h = 60 - z$.

TABLE 6-2. INPUT DATA SET FOR THE TWO-DIMENSIONAL 3DFEMWATER PROBLEM

```
   2 SIMULATION OF TWO-D STEADY DRAINAGE; L=M, T=DAY, M=KG                    111
C ******* DATA SET 2:  BASIC INTEGERS
   242    100    1      0      0      0      6      1      0      0      50     20     1      100
C ******* DATA SET 3:  BASIC REAL PARAMETERS
   0.05D0       0.2D0      1.0D0      20.0D0     2.0D-3     2.0D-3     1.0D0      7.316D10
   1.1232D4     1.0D0      0.5D0      0.5D0      0.0
C ******* DATA SET 4:  PRINTER, STORAGE CONTROL AND TIME STEP SIZE RESETTING
33
11
   1.0D38
C ******* DATA SET 5:  MATERIAL PROPERTIES
   0.31D0       0.0D0      0.12D0     0.0D0      0.0D0      0.0D0
C ******* DATA SET 6:  SOIL PROPERTY PARAMETERS
   0      5      0
   0.100D0      0.390D0    0.00D0     0.059D0    1.48D0                THPROP
C ******* DATA SET 7:  NODE COORDINATES
     1     10     11          0.0D0      0.0D0      0.0D0      1.0D0      0.0D0      0.0D0
     2     10     11          0.0D0      0.0D0      1.0D0      1.0D0      0.0D0      0.0D0
     3     10     11          0.0D0      0.0D0      2.0D0      1.0D0      0.0D0      0.0D0
     4     10     11          0.0D0      0.0D0      3.0D0      1.0D0      0.0D0      0.0D0
     5     10     11          0.0D0      0.0D0      4.0D0      1.0D0      0.0D0      0.0D0
     6     10     11          0.0D0      0.0D0      5.0D0      1.0D0      0.0D0      0.0D0
     7     10     11          0.0D0      0.0D0      6.0D0      1.0D0      0.0D0      0.0D0
     8     10     11          0.0D0      0.0D0      7.0D0      1.0D0      0.0D0      0.0D0
     9     10     11          0.0D0      0.0D0      8.0D0      1.0D0      0.0D0      0.0D0
    10     10     11          0.0D0      0.0D0      9.0D0      1.0D0      0.0D0      0.0D0
    11     10     11          0.0D0      0.0D0      10.0D0     1.0D0      0.0D0      0.0D0
   122     10     11          0.0D0      10.0D0     0.0D0      1.0D0      0.0D0      0.0D0
   123     10     11          0.0D0      10.0D0     1.0D0      1.0D0      0.0D0      0.0D0
   124     10     11          0.0D0      10.0D0     2.0D0      1.0D0      0.0D0      0.0D0
   125     10     11          0.0D0      10.0D0     3.0D0      1.0D0      0.0D0      0.0D0
   126     10     11          0.0D0      10.0D0     4.0D0      1.0D0      0.0D0      0.0D0
   127     10     11          0.0D0      10.0D0     5.0D0      1.0D0      0.0D0      0.0D0
   128     10     11          0.0D0      10.0D0     6.0D0      1.0D0      0.0D0      0.0D0
   129     10     11          0.0D0      10.0D0     7.0D0      1.0D0      0.0D0      0.0D0
   130     10     11          0.0D0      10.0D0     8.0D0      1.0D0      0.0D0      0.0D0
   131     10     11          0.0D0      10.0D0     9.0D0      1.0D0      0.0D0      0.0D0
   132     10     11          0.0D0      10.0D0     10.0D0     1.0D0      0.0D0      0.0D0
     0      0      0          0.0        0.0        0.0        0.0        0.0        0.0
C ******* DATA SET 8: SUBREGIONAL DATA
   2
   1      1      1      121      0
   0      0      0      0        0    END OF NNPLR(K)
   1      120    1      1        1
   0      0      0      0        0    END OF GNLR(I,1)
   1      120    1      122      1
   0      0      0      0        0    END OF GNLR(I,2)
```

TABLE 6-2. INPUT DATA SET FOR THE TWO-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

```
C ******* DATA SET 9: ELEMENT INCIDENCES
  1   9   1    1   12  133  122    2   13  134  123  1
 11   9   1   12   23  144  133   13   24  145  134  1
 21   9   1   23   34  155  144   24   35  156  145  1
 31   9   1   34   45  166  155   35   46  167  156  1
 41   9   1   45   56  177  166   46   57  178  167  1
 51   9   1   56   67  188  177   57   68  189  178  1
 61   9   1   67   78  199  188   68   79  200  189  1
 71   9   1   78   89  210  199   79   90  211  200  1
 81   9   1   89  100  221  210   90  101  222  211  1
 91   9   1  100  111  232  221  101  112  233  222  1
  0   0   0    0    0    0    0    0    0    0    0  0 END OF
IE
C ******* DATA SET 11:  INITITAL CONDITIONS
  1  10  11  10.0D0   0.0D0   0.0D0
  2  10  11   9.0D0   0.0D0   0.0D0
  3  10  11   8.0D0   0.0D0   0.0D0
  4  10  11   7.0D0   0.0D0   0.0D0
  5  10  11   6.0D0   0.0D0   0.0D0
  6  10  11   5.0D0   0.0D0   0.0D0
  7  10  11   4.0D0   0.0D0   0.0D0
  8  10  11   3.0D0   0.0D0   0.0D0
  9  10  11   2.0D0   0.0D0   0.0D0
 10  10  11   1.0D0   0.0D0   0.0D0
 11  10  11   0.0D0   0.0D0   0.0D0
122  10  11  10.0D0   0.0D0   0.0D0
123  10  11   9.0D0   0.0D0   0.0D0
124  10  11   8.0D0   0.0D0   0.0D0
125  10  11   7.0D0   0.0D0   0.0D0
126  10  11   6.0D0   0.0D0   0.0D0
127  10  11   5.0D0   0.0D0   0.0D0
128  10  11   4.0D0   0.0D0   0.0D0
129  10  11   3.0D0   0.0D0   0.0D0
130  10  11   2.0D0   0.0D0   0.0D0
131  10  11   1.0D0   0.0D0   0.0D0
132  10  11   0.0D0   0.0D0   0.0D0
  0   0   0   0.0D0   0.0D0   0.0D0      END OF IC
C ******* DATA SET 12:  SOURCE/SINK AND B. C. CONTROL INTEGERS
  0   0   0   0   0   0   0   0   6   1   2   0
 18  38   2   2   0   0   0   0   0   0   0   0   0   0   0
```

TABLE 6-2. INPUT DATA SET FOR THE TWO-DIMENSIONAL 3DFEMWATER PROBLEM (concluded)

```
C ******* DATA SET 14: VARIABLE BOUNDARY CONDITIONS
  0.0D0        6.0D-3        1.0D38        6.0D-3
  0.0D0        0.0D00        1.0D38        0.0D00
      1   9        1   1        0
     11   7        1   2        0
      0   0        0   0        0                    END OF IRTYP
      1   9        1  11       22     143     132    11    11    11    11
     11   7        1 120      241     242     121    -1    -1    -1    -1
      0   0        0   0        0       0       0     0     0     0     0    END OF ISV(J,I) J=1,4
      1  10        1  11       11
     12   7        1 120       -1
     20  10        1 132       11
     31   7        1 241       -1
      0   0        0   0        0              END OF NPVB
      1  37        1            0.0D0         0.0D0         0.0D0
      0   0        0            0.0D0         0.0D0         0.0D0          END OF HCON
      1  37        1           -90.0D2        0.0D0         0.0D0
      0   0        0            0.0D0         0.0D0         0.0D0          END OF HMIN
C ******* DATA SET 15: DIRICHLET BOUNDARY CONDITIONS
       0.0D0        2.0D0        1.0D38        2.0D0
    111  112  113  232   233  234
      1    5    1    1     0
      0    0    0    0     0 END OF IDTYP
      0              END OF JOB ----------------------------------------------------------------------------000
```

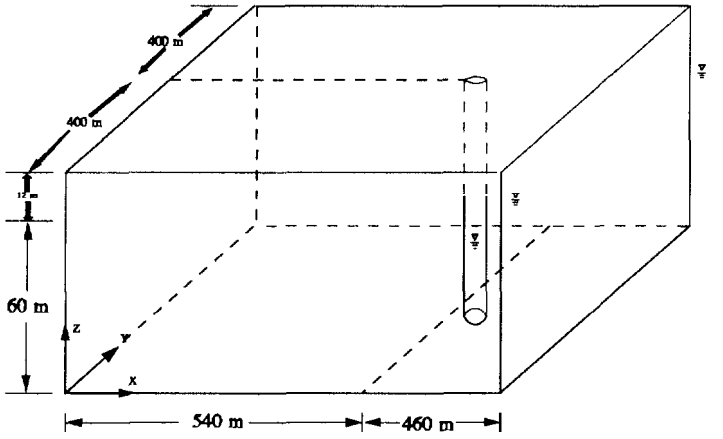


Figure 6.3. Three-dimensional steady-state flow to a pumping well.

The region of interest is discretized with 20 x 8 x 10 = 1600 elements, resulting in 21 x 9 x 11 = 2079 nodal points. The nodes are located at x = 0, 70, 120, 160, 200, 275, 350, 400, 450, 500, 540, 570, 600, 650, 750, 800, 850, 900, 950, and 1000 in the x-direction, and at z = 0, 15, 30, 35, 40, 45, 50, 55, 60, 66, and 72 in the z-direction. In the y-direction, nodes are spaced evenly at Az = 50 m. For the simulation, each of the nine vertical planes perpendicular to the y-axis is considered a subregion. Thus, a total of 9 subregions, each with 231 node points, is used for the subregional block iteration simulation.

The pressure head tolerance is set at .01 m for the nonlinear iteration and is .005 m for the block iteration. The relaxation factors for the nonlinear iteration and block iteration are set equal to 1.0 and 1.5, respectively.

The input data set for this problem, prepared according to the instructions in Sections 4.1 and 5.1, is shown in Table 6-3.

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM

```
   3 SIMULATION OF THREE-D PUMPING WELL; L = M, T = DAY, M = KG                  011
C ******* DATA SET 2:  BASIC INTEGER PARAMETERS
 2079 1600   1   0   0   0   6   1   0   0  50  20   1 100
C ******* DATA SET 3:  BASIC REAL PARAMETERS
      0.05D0      0.0D0    1.0D0   20.0D0   1.0D-2   1.0D-2   1.0D0   7.316D10
      1. 1232D4  1.0D0    1.0D0    1.5D0
C ******* DATA SET 4:  PRINTER, STORAGE CONTROL AND TIME STEP SIZE RESETTING
55
11
      1.0D38
C ******* DATA SET 5:  MATERIAL PROPERTIES
      0.31D0  0.03D0      0.12D0   0.0D0   0.0D0   0.0D0
C ******* DATA SET 6: SOIL PROPERTY PARAMETERS
      0   5   0
      0.1000D0     0.390D0     0.00D0     0.059D0    1.48D0            THPROP
C ******* DATA SET 7: NODE COORDINATES
    1   8   231     0.00D+00    0.00D+00    0.00D+00    0.00D+00    0.50D+02    0.00D+00
    2   8   231     0.00D+00    0.00D+00    0.15D+02    0.00D+00    0.50D+02    0.00D+00
    3   8   231     0.00D+00    0.00D+00    0.30D+02    0.00D+00    0.50D+02    0.00D+00
    4   8   231     0.00D+00    0.00D+00    0.35D+02    0.00D+00    0.50D+02    0.00D+00
    5   8   231     0.00D+00    0.00D+00    0.40D+02    0.00D+00    0.50D+02    0.00D+00
    6   8   231     0.00D+00    0.00D+00    0.45D+02    0.00D+00    0.50D+02    0.00D+00
    7   8   231     0.00D+00    0.00D+00    0.50D+02    0.00D+00    0.50D+02    0.00D+00
    8   8   231     0.00D+00    0.00D+00    0.55D+02    0.00D+00    0.50D+02    0.00D+00
    9   8   231     0.00D+00    0.00D+00    0.60D+02    0.00D+00    0.50D+02    0.00D+00
   10   8   231     0.00D+00    0.00D+00    0.66D+02    0.00D+00    0.50D+02    0.00D+00
   11   8   231     0.00D+00    0.00D+00    0.72D+02    0.00D+00    0.50D+02    0.00D+00
   12   8   231     0.70D+02    0.00D+00    0.00D+00    0.00D+00    0.50D+02    0.00D+00
   13   8   231     0.70D+02    0.00D+00    0.15D+02    0.00D+00    0.50D+02    0.00D+00
   14   8   231     0.70D+02    0.00D+00    0.30D+02    0.00D+00    0.50D+02    0.00D+00
   15   8   231     0.70D+02    0.00D+00    0.35D+02    0.00D+00    0.50D+02    0.00D+00
   16   8   231     0.70D+02    0.00D+00    0.40D+02    0.00D+00    0.50D+02    0.00D+00
   17   8   231     0.70D+02    0.00D+00    0.45D+02    0.00D+00    0.50D+02    0.00D+00
   18   8   231     0.70D+02    0.00D+00    0.50D+02    0.00D+00    0.50D+02    0.00D+00
   19   8   231     0.70D+02    0.00D+00    0.55D+02    0.00D+00    0.50D+02    0.00D+00
   20   8   231     0.70D+02    0.00D+00    0.60D+02    0.00D+00    0.50D+02    0.00D+00
   21   8   231     0.70D+02    0.00D+00    0.66D+02    0.00D+00    0.50D+02    0.00D+00
   22   8   231     0.70D+02    0.00D+00    0.72D+02    0.00D+00    0.50D+02    0.00D+00
   23   8   231     0.12D+03    0.00D+00    0.00D+00    0.00D+00    0.50D+02    0.00D+00
   24   8   231     0.12D+03    0.00D+00    0.15D+00    0.00D+00    0.50D+02    0.00D+00
   25   8   231     0.12D+03    0.00D+00    0.30D+00    0.00D+00    0.50D+02    0.00D+00
   26   8   231     0.12D+03    0.00D+00    0.35D+02    0.00D+00    0.50D+02    0.00D+00
   27   8   231     0.12D+03    0.00D+00    0.40D+02    0.00D+00    0.50D+02    0.00D+00
   28   8   231     0.12D+03    0.00D+00    0.45D+02    0.00D+00    0.50D+02    0.00D+00
   29   8   231     0.12D+03    0.00D+00    0.50D+02    0.00D+00    0.50D+02    0.00D+00
   30   8   231     0.12D+03    0.00D+00    0.55D+02    0.00D+00    0.50D+02    0.00D+00
   31   8   231     0.12D+03    0.00D+00    0.60D+02    0.00D+00    0.50D+02    0.00D+00
   32   8   231     0.12D+03    0.00D+00    0.66D+02    0.00D+00    0.50D+02    0.00D+00
   33   8   231     0.12D+03    0.00D+00    0.72D+02    0.00D+00    0.50D+02    0.00D+00
   34   8   231     0.16D+03    0.00D+00    0.00D+00    0.00D+00    0.50D+02    0.00D+00
```

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

35	8	231	0.16D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
36	8	231	0.16D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
37	8	231	0.16D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
38	8	231	0.16D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
39	8	231	0.16D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
40	8	231	0.16D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
41	8	231	0.16D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
42	8	231	0.16D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
43	8	231	0.16D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
44	8	231	0.16D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
45	8	231	0.20D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
46	8	231	0.20D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
47	8	231	0.20D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
48	8	231	0.20D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
49	8	231	0.20D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
50	8	231	0.20D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
51	8	231	0.20D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
52	8	231	0.20D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
53	8	231	0.20D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
54	8	231	0.20D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
55	8	231	0.20D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
56	8	231	0.28D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
57	8	231	0.28D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
58	8	231	0.28D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
59	8	231	0.28D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
60	8	231	0.28D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
61	8	231	0.28D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
62	8	231	0.28D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
63	8	231	0.28D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
64	8	231	0.28D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
65	8	231	0.28D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
66	8	231	0.28D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
67	8	231	0.35D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
68	8	231	0.35D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
69	8	231	0.35D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
70	8	231	0.35D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
71	8	231	0.35D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
72	8	231	0.35D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
73	8	231	0.35D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
74	8	231	0.35D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
75	8	231	0.35D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
76	8	231	0.35D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
77	8	231	0.35D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
78	8	231	0.40D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
79	8	231	0.40D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
80	8	231	0.40D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
81	8	231	0.40D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
82	8	231	0.40D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
83	8	231	0.40D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
84	8	231	0.40D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

85	8	231	0.40D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
86	8	231	0.40D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
87	8	231	0.40D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
88	8	231	0.40D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
89	8	231	0.45D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
90	8	231	0.45D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
91	8	231	0.45D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
92	8	231	0.45D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
93	8	231	0.45D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
94	8	231	0.45D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
95	8	231	0.45D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
96	8	231	0.45D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
97	8	231	0.45D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
98	8	231	0.45D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
99	8	231	0.45D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
100	8	231	0.50D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
101	8	231	0.50D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
102	8	231	0.50D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
103	8	231	0.50D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
104	8	231	0.50D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
105	8	231	0.50D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
106	8	231	0.50D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
107	8	231	0.50D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
108	8	231	0.50D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
109	8	231	0.50D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
110	8	231	0.50D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
111	8	231	0.54D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
112	8	231	0.54D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
113	8	231	0.54D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
114	8	231	0.54D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
115	8	231	0.54D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
116	8	231	0.54D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
117	8	231	0.54D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
118	8	231	0.54D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
119	8	231	0.54D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
120	8	231	0.54D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
121	8	231	0.54D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
122	8	231	0.57D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
123	8	231	0.57D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
124	8	231	0.57D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
125	8	231	0.57D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
126	8	231	0.57D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
127	8	231	0.57D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
128	8	231	0.57D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
129	8	231	0.57D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
130	8	231	0.57D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
131	8	231	0.57D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
132	8	231	0.57D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
133	8	231	0.60D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
134	8	231	0.60D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

135	8	231	0.60D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
136	8	231	0.60D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
137	8	231	0.60D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
138	8	231	0.60D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
139	8	231	0.60D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
140	8	231	0.60D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
141	8	231	0.60D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
142	8	231	0.60D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
143	8	231	0.60D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
144	8	231	0.65D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
145	8	231	0.65D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
146	8	231	0.65D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
147	8	231	0.65D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
148	8	231	0.65D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
149	8	231	0.65D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
150	8	231	0.65D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
151	8	231	0.65D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
152	8	231	0.65D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
153	8	231	0.65D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
154	8	231	0.65D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
155	8	231	0.70D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
156	8	231	0.70D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
157	8	231	0.70D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
158	8	231	0.70D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
159	8	231	0.70D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
160	8	231	0.70D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
161	8	231	0.70D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
162	8	231	0.70D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
163	8	231	0.70D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
164	8	231	0.70D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
165	8	231	0.70D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
166	8	231	0.75D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
167	8	231	0.75D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
168	8	231	0.75D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
169	8	231	0.75D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
170	8	231	0.75D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
171	8	231	0.75D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
172	8	231	0.75D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
173	8	231	0.75D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
174	8	231	0.75D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
175	8	231	0.75D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
176	8	231	0.75D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
177	8	231	0.80D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
178	8	231	0.80D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
179	8	231	0.80D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
180	8	231	0.80D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
181	8	231	0.80D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
182	8	231	0.80D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
183	8	231	0.80D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
184	8	231	0.80D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

185	8	231	0.80D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
186	8	231	0.80D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
187	8	231	0.80D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
188	8	231	0.85D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
189	8	231	0.85D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
190	8	231	0.85D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
191	8	231	0.85D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
192	8	231	0.85D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
193	8	231	0.85D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
194	8	231	0.85D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
195	8	231	0.85D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
196	8	231	0.85D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
197	8	231	0.85D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
198	8	231	0.85D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
199	8	231	0.90D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
200	8	231	0.90D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
201	8	231	0.90D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
202	8	231	0.90D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
203	8	231	0.90D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
204	8	231	0.90D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
205	8	231	0.90D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
206	8	231	0.90D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
207	8	231	0.90D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
208	8	231	0.90D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
209	8	231	0.90D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
210	8	231	0.95D+03	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
211	8	231	0.95D+03	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
212	8	231	0.95D+03	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
213	8	231	0.95D+03	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
214	8	231	0.95D+03	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
215	8	231	0.95D+03	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
216	8	231	0.95D+03	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
217	8	231	0.95D+03	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
218	8	231	0.95D+03	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
219	8	231	0.95D+03	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
220	8	231	0.95D+03	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
221	8	231	0.10D+04	0.00D+00	0.00D+00	0.00D+00	0.50D+02	0.00D+00
222	8	231	0.10D+04	0.00D+00	0.15D+02	0.00D+00	0.50D+02	0.00D+00
223	8	231	0.10D+04	0.00D+00	0.30D+02	0.00D+00	0.50D+02	0.00D+00
224	8	231	0.10D+04	0.00D+00	0.35D+02	0.00D+00	0.50D+02	0.00D+00
225	8	231	0.10D+04	0.00D+00	0.40D+02	0.00D+00	0.50D+02	0.00D+00
226	8	231	0.10D+04	0.00D+00	0.45D+02	0.00D+00	0.50D+02	0.00D+00
227	8	231	0.10D+04	0.00D+00	0.50D+02	0.00D+00	0.50D+02	0.00D+00
228	8	231	0.10D+04	0.00D+00	0.55D+02	0.00D+00	0.50D+02	0.00D+00
229	8	231	0.10D+04	0.00D+00	0.60D+02	0.00D+00	0.50D+02	0.00D+00
230	8	231	0.10D+04	0.00D+00	0.66D+02	0.00D+00	0.50D+02	0.00D+00
231	8	231	0.10D+04	0.00D+00	0.72D+02	0.00D+00	0.50D+02	0.00D+00
0	0	0	0.0		0.0	0.0	0.0	0.00.0

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

```
C ******* DATA SET 8: SUBREGIONAL  DATA
      9
      1     8     1     231     0
      0     0     0     0       0          END OF NNPLR(9)
      1     230   1     1       1
      0     0     0     0       0          END OF GNLR(I,1)
      1     230   1     232     1
      0     0     0     0       0          END OF GNLR(I,2)
      1     230   1     463     1
      0     0     0     0       0          END OF GNLR(I,3)
      1     230   1     694     1
      0     0     0     0       0          END OF GNLR(I,4)
      1     230   1     925     1
      0     0     0     0       0          END OF GNLR(I,5)
      1     230   1     1156    1
      0     0     0     0       0          END OF GNLR(I,6)
      1     230   1     1387    1
      0     0     0     0       0          END OF GNLR(I,7)
      1     230   1     1618    1
      0     0     0     0       0          END OF GNLR(I,8)
      1     230   1     1849    1
      0     0     0     0       0          END OF GNLR(I,9)
C ******** DATA SET 10: ELEMENT INCIDENCES
      1     9     1     1     12    243   232   2     13    244   233   1
     11     9     1     12    23    254   243   13    24    255   244   1
     21     9     1     23    34    265   254   24    35    266   255   1
     31     9     1     34    45    276   265   35    46    277   266   1
     41     9     1     45    56    287   276   46    57    288   277   1
     51     9     1     56    67    298   287   57    68    299   288   1
     61     9     1     67    78    309   298   68    79    310   299   1
     71     9     1     78    89    320   309   79    90    321   310   1
     81     9     1     89    100   331   320   90    101   332   321   1
     91     9     1     100   111   342   331   101   112   343   332   1
    101     9     1     111   122   353   342   112   123   354   343   1
    111     9     1     122   133   364   353   123   134   365   354   1
    121     9     1     133   144   375   364   134   145   376   365   1
    131     9     1     144   155   386   375   145   156   387   376   1
    141     9     1     155   166   397   386   156   167   398   387   1
    151     9     1     166   177   408   397   167   178   409   398   1
    161     9     1     177   188   419   408   178   189   420   409   1
    171     9     1     188   199   430   419   189   200   431   420   1
    181     9     1     199   210   441   430   200   211   442   431   1
    191     9     1     210   221   452   441   211   222   453   442   1
    201     9     1     232   243   474   463   233   244   475   464   1
    211     9     1     243   254   485   474   244   255   486   475   1
    221     9     1     254   265   496   485   255   266   497   486   1
    231     9     1     265   276   507   496   266   277   508   497   1
    241     9     1     276   287   518   507   277   288   519   508   1
    251     9     1     287   298   529   518   288   299   530   519   1
    261     9     1     298   309   540   529   299   310   541   530   1
```

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

271	9	1	309	320	551	540	310	321	552	541	1
281	9	1	320	331	562	551	321	332	563	552	1
291	9	1	331	342	573	562	332	343	574	563	1
301	9	1	342	353	584	573	343	354	585	574	1
311	9	1	353	364	595	584	354	365	596	585	1
321	9	1	364	375	606	595	365	376	607	596	1
331	9	1	375	386	617	606	376	387	618	607	1
341	9	1	386	397	628	617	387	398	629	618	1
351	9	1	397	408	639	628	398	409	640	629	1
361	9	1	408	419	650	639	409	420	651	640	1
371	9	1	419	430	661	650	420	431	662	651	1
381	9	1	430	441	672	661	431	442	673	662	1
391	9	1	441	452	683	672	442	453	684	673	1
401	9	1	463	474	705	694	464	475	706	695	1
411	9	1	474	485	716	705	475	486	717	706	1
421	9	1	485	496	727	716	486	497	728	717	1
431	9	1	496	507	738	727	497	508	739	728	1
441	9	1	507	518	749	738	508	519	750	739	1
451	9	1	518	529	760	749	519	530	761	750	1
461	9	1	529	540	771	760	530	541	772	761	1
471	9	1	540	551	782	771	541	552	783	772	1
481	9	1	551	562	793	782	552	563	794	783	1
491	9	1	562	573	804	793	563	574	805	794	1
501	9	1	573	584	815	804	574	585	816	805	1
511	9	1	584	595	826	815	585	596	827	816	1
521	9	1	595	606	837	826	596	607	838	827	1
531	9	1	606	617	848	837	607	618	849	838	1
541	9	1	617	628	859	848	618	629	860	849	1
551	9	1	628	639	870	859	629	640	871	860	1
561	9	1	639	650	881	870	640	651	882	871	1
571	9	1	650	661	892	881	651	662	893	882	1
581	9	1	661	672	903	892	662	673	904	893	1
591	9	1	672	683	914	903	673	684	915	904	1
601	9	1	694	705	936	925	695	706	937	926	1
611	9	1	705	716	947	936	706	717	948	937	1
621	9	1	716	727	958	947	717	728	959	948	1
631	9	1	727	738	969	958	728	739	970	959	1
641	9	1	738	749	980	969	739	750	981	970	1
651	9	1	749	760	991	980	750	761	992	981	1
661	9	1	760	771	1002	991	761	772	1003	992	1
671	9	1	771	782	1013	1002	772	783	1014	1003	1
681	9	1	782	793	1024	1013	783	794	1025	1014	1
691	9	1	793	804	1035	1024	794	805	1036	1025	1
701	9	1	804	815	1046	1035	805	816	1047	1036	1
711	9	1	815	826	1057	1046	816	827	1058	1047	1
721	9	1	826	837	1068	1057	827	838	1069	1058	1
731	9	1	837	848	1079	1068	838	849	1080	1069	1
741	9	1	848	859	1090	1079	849	860	1091	1080	1
751	9	1	859	870	1101	1090	860	871	1102	1091	1
761	9	1	870	881	1112	1101	871	882	1113	1102	1

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

771	9	1	881	892	1123	1112	882	893	1124	1113	1
781	9	1	892	903	1134	1123	893	904	1135	1124	1
791	9	1	903	914	1145	1134	904	915	1146	1135	1
801	9	1	925	936	1167	1156	926	937	1168	1157	1
811	9	1	936	947	1178	1167	937	948	1179	1168	1
821	9	1	947	958	1189	1178	948	959	1190	1179	1
831	9	1	958	969	1200	1189	959	970	1201	1190	1
841	9	1	969	980	1211	1200	970	981	1212	1201	1
851	9	1	980	991	1222	1211	981	992	1223	1212	1
861	9	1	991	1002	1233	1222	992	1003	1234	1223	1
871	9	1	1002	1013	1244	1233	1003	1014	1245	1234	1
881	9	1	1013	1024	1255	1244	1014	1025	1256	1245	1
891	9	1	1024	1035	1266	1255	1025	1036	1267	1256	1
901	9	1	1035	1046	1277	1266	1036	1047	1278	1267	1
911	9	1	1046	1057	1288	1277	1047	1058	1289	1278	1
921	9	1	1057	1068	1299	1288	1058	1069	1300	1289	1
931	9	1	1068	1079	1310	1299	1069	1080	1311	1300	1
941	9	1	1079	1090	1321	1310	1080	1091	1322	1311	1
951	9	1	1090	1101	1332	1321	1091	1102	1333	1322	1
961	9	1	1101	1112	1343	1332	1102	1113	1344	1333	1
971	9	1	1112	1123	1354	1343	1113	1124	1355	1344	1
981	9	1	1123	1134	1365	1354	1124	1135	1366	1355	1
991	9	1	1134	1145	1376	1365	1135	1146	1377	1366	1
1001	9	1	1156	1167	1398	1387	1157	1168	1399	1388	1
1011	9	1	1167	1178	1409	1398	1168	1179	1410	1399	1
1021	9	1	1178	1189	1420	1409	1179	1190	1421	1410	1
1031	9	1	1189	1200	1431	1420	1190	1201	1432	1421	1
1041	9	1	1200	1211	1442	1431	1201	1212	1443	1432	1
1051	9	1	1211	1222	1453	1442	1212	1223	1454	1443	1
1061	9	1	1222	1233	1464	1453	1223	1234	1465	1454	1
1071	9	1	1233	1244	1475	1464	1234	1245	1476	1465	1
1081	9	1	1244	1255	1486	1475	1245	1256	1487	1476	1
1091	9	1	1255	1266	1497	1486	1256	1267	1498	1487	1
1101	9	1	1266	1277	1508	1497	1267	1278	1509	1498	1
1111	9	1	1277	1288	1519	1508	1278	1289	1520	1509	1
1121	9	1	1288	1299	1530	1519	1289	1300	1531	1520	1
1131	9	1	1299	1310	1541	1530	1300	1311	1542	1531	1
1141	9	1	1310	1321	1552	1541	1311	1322	1553	1542	1
1151	9	1	1321	1332	1563	1552	1322	1333	1564	1553	1
1161	9	1	1332	1343	1574	1563	1333	1344	1575	1564	1
1171	9	1	1343	1354	1585	1574	1344	1355	1586	1575	1
1181	9	1	1354	1365	1596	1585	1355	1366	1597	1586	1
1191	9	1	1365	1376	1607	1596	1366	1377	1608	1597	1
1201	9	1	1387	1398	1629	1618	1388	1399	1630	1619	1
1211	9	1	1398	1409	1640	1629	1399	1410	1641	1630	1
1221	9	1	1409	1420	1651	1640	1410	1421	1652	1641	1
1231	9	1	1420	1431	1662	1651	1421	1432	1663	1652	1
1241	9	1	1431	1442	1673	1662	1432	1443	1674	1663	1
1251	9	1	1442	1453	1684	1673	1443	1454	1685	1674	1
1261	9	1	1453	1464	1695	1684	1454	1465	1696	1685	1

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

```
 1271   9   1  1464  1475  1706  1695  1465  1476  1707  1696  1
 1281   9   1  1475  1486  1717  1706  1476  1487  1718  1707  1
 1291   9   1  1486  1497  1728  1717  1487  1498  1729  1718  1
 1301   9   1  1497  1508  1739  1728  1498  1509  1740  1729  1
 1311   9   1  1508  1519  1750  1739  1509  1520  1751  1740  1
 1321   9   1  1519  1530  1761  1750  1520  1531  1762  1751  1
 1331   9   1  1530  1541  1772  1761  1531  1542  1773  1762  1
 1341   9   1  1541  1552  1783  1772  1542  1553  1784  1773  1
 1351   9   1  1552  1563  1794  1783  1553  1564  1795  1784  1
 1361   9   1  1563  1574  1805  1794  1564  1575  1806  1795  1
 1371   9   1  1574  1585  1816  1805  1575  1586  1817  1806  1
 1381   9   1  1585  1596  1827  1816  1586  1597  1828  1817  1
 1391   9   1  1596  1607  1838  1827  1597  1608  1839  1828  1
 1401   9   1  1618  1629  1860  1849  1619  1630  1861  1850  1
 1411   9   1  1629  1640  1871  1860  1630  1641  1872  1861  1
 1421   9   1  1640  1651  1882  1871  1641  1652  1883  1872  1
 1431   9   1  1651  1662  1893  1882  1652  1663  1894  1883  1
 1441   9   1  1662  1673  1904  1893  1663  1674  1905  1894  1
 1451   9   1  1673  1684  1915  1904  1674  1685  1916  1905  1
 1461   9   1  1684  1695  1926  1915  1685  1696  1927  1916  1
 1471   9   1  1695  1706  1937  1926  1696  1707  1938  1927  1
 1481   9   1  1706  1717  1948  1937  1707  1718  1949  1938  1
 1491   9   1  1717  1728  1959  1948  1718  1729  1960  1949  1
 1501   9   1  1728  1739  1970  1959  1729  1740  1971  1960  1
 1511   9   1  1739  1750  1981  1970  1740  1751  1982  1971  1
 1521   9   1  1750  1761  1992  1981  1751  1762  1993  1982  1
 1531   9   1  1761  1772  2003  1992  1762  1773  2004  1993  1
 1541   9   1  1772  1783  2014  2003  1773  1784  2015  2004  1
 1551   9   1  1783  1794  2025  2014  1784  1795  2026  2015  1
 1561   9   1  1794  1805  2036  2025  1795  1806  2037  2026  1
 1571   9   1  1805  1816  2047  2036  1806  1817  2048  2037  1
 1581   9   1  1816  1827  2058  2047  1817  1828  2059  2048  1
 1591   9   1  1827  1838  2069  2058  1828  1839  2070  2059  1
    0   0   0     0     0     0     0     0     0     0     0  0 END OF IE
C ******* DATA SET 11:  INITIAL CONDITIONS
    1   8 231   0.60D+02   0.00D+00   0.0
    2   8 231   0.45D+02   0.00D+00   0.0
    3   8 231   0.30D+02   0.00D+00   0.0
    4   8 231   0.25D+02   0.00D+00   0.0
    5   8 231   0.20D+02   0.00D+00   0.0
    6   8 231   0.15D+02   0.00D+00   0.0
    7   8 231   0.10D+02   0.00D+00   0.0
    8   8 231   0.50D+01   0.00D+00   0.0
    9   8 231   0.00D+00   0.00D+00   0.0
   10   8 231  -0.60D+01   0.00D+00   0.0
   11   8 231  -0.12D+02   0.00D+00   0.0
   12   8 231   0.60D+02   0.00D+00   0.0
   13   8 231   0.45D+02   0.00D+00   0.0
   14   8 231   0.30D+02   0.00D+00   0.0
   15   8 231   0.25D+02   0.00D+00   0.0
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TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

16	8	231	0.20D+02	0.00D+00	0.0
17	8	231	0.15D+02	0.00D+00	0.0
18	8	231	0.10D+02	0.00D+00	0.0
19	8	231	0.50D+01	0.00D+00	0.0
20	8	231	0.00D+00	0.00D+00	0.0
21	8	231	-0.60D+01	0.00D+00	0.0
22	8	231	-0.12D+02	0.00D+00	0.0
23	8	231	0.60D+02	0.00D+00	0.0
24	8	231	0.45D+02	0.00D+00	0.0
25	8	231	0.30D+02	0.00D+00	0.0
26	8	231	0.25D+02	0.00D+00	0.0
27	8	231	0.20D+02	0.00D+00	0.0
28	8	231	0.15D+02	0.00D+00	0.0
29	8	231	0.10D+02	0.00D+00	0.0
30	8	231	0.50D+01	0.00D+00	0.0
31	8	231	0.00D+00	0.00D+00	0.0
32	8	231	-0.60D+01	0.00D+00	0.0
33	8	231	-0.12D+02	0.00D+00	0.0
34	8	231	0.60D+02	0.00D+00	0.0
35	8	231	0.45D+02	0.00D+00	0.0
36	8	231	0.30D+02	0.00D+00	0.0
37	8	231	0.25D+02	0.00D+00	0.0
38	8	231	0.20D+02	0.00D+00	0.0
39	8	231	0.15D+02	0.00D+00	0.0
40	8	231	0.10D+02	0.00D+00	0.0
41	8	231	0.50D+01	0.00D+00	0.0
42	8	231	0.00D+00	0.00D+00	0.0
43	8	231	-0.60D+01	0.00D+00	0.0
44	8	231	-0.12D+02	0.00D+00	0.0
45	8	231	0.60D+02	0.00D+00	0.0
46	8	231	0.45D+02	0.00D+00	0.0
47	8	231	0.30D+02	0.00D+00	0.0
48	8	231	0.25D+02	0.00D+00	0.0
49	8	231	0.20D+02	0.00D+00	0.0
50	8	231	0.15D+02	0.00D+00	0.0
51	8	231	0.10D+02	0.00D+00	0.0
52	8	231	0.50D+01	0.00D+00	0.0
53	8	231	0.00D+00	0.00D+00	0.0
54	8	231	-0.60D+01	0.00D+00	0.0
55	8	231	-0.12D+02	0.00D+00	0.0
56	8	231	0.60D+02	0.00D+00	0.0
57	8	231	0.45D+02	0.00D+00	0.0
58	8	231	0.30D+02	0.00D+00	0.0
59	8	231	0.25D+02	0.00D+00	0.0
60	8	231	0.20D+02	0.00D+00	0.0
61	8	231	0.15D+02	0.00D+00	0.0
62	8	231	0.10D+02	0.00D+00	0.0
63	8	231	0.50D+01	0.00D+00	0.0
64	8	231	0.00D+00	0.00D+00	0.0
65	8	231	-0.60D+01	0.00D+00	0.0

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

66	8	231	-0.12D+02	0.00D+00	0.0
67	8	231	0.60D+02	0.00D+00	0.0
68	8	231	0.45D+02	0.00D+00	0.0
69	8	231	0.30D+02	0.00D+00	0.0
70	8	231	0.25D+02	0.00D+00	0.0
71	8	231	0.20D+02	0.00D+00	0.0
72	8	231	0.15D+02	0.00D+00	0.0
73	8	231	0.10D+02	0.00D+00	0.0
74	8	231	0.50D+01	0.00D+00	0.0
75	8	231	0.00D+00	0.00D+00	0.0
76	8	231	-0.60D+01	0.00D+00	0.0
77	8	231	-0.12D+02	0.00D+00	0.0
78	8	231	0.60D+02	0.00D+00	0.0
79	8	231	0.45D+02	0.00D+00	0.0
80	8	231	0.30D+02	0.00D+00	0.0
81	8	231	0.25D+02	0.00D+00	0.0
82	8	231	0.20D+02	0.00D+00	0.0
83	8	231	0.15D+02	0.00D+00	0.0
84	8	231	0.10D+02	0.00D+00	0.0
85	8	231	0.50D+01	0.00D+00	0.0
86	8	231	0.00D+00	0.00D+00	0.0
87	8	231	-0.60D+01	0.00D+00	0.0
88	8	231	-0.12D+02	0.00D+00	0.0
89	8	231	0.60D+02	0.00D+00	0.0
90	8	231	0.45D+02	0.00D+00	0.0
91	8	231	0.30D+02	0.00D+00	0.0
92	8	231	0.25D+02	0.00D+00	0.0
93	8	231	0.20D+02	0.00D+00	0.0
94	8	231	0.15D+02	0.00D+00	0.0
95	8	231	0.10D+02	0.00D+00	0.0
96	8	231	0.50D+01	0.00D+00	0.0
97	8	231	0.00D+00	0.00D+00	0.0
98	8	231	-0.60D+01	0.00D+00	0.0
99	8	231	-0.12D+02	0.00D+00	0.0
100	8	231	0.60D+02	0.00D+00	0.0
101	8	231	0.45D+02	0.00D+00	0.0
102	8	231	0.30D+02	0.00D+00	0.0
103	8	231	0.25D+02	0.00D+00	0.0
104	8	231	0.20D+02	0.00D+00	0.0
105	8	231	0.15D+02	0.00D+00	0.0
106	8	231	0.10D+02	0.00D+00	0.0
107	8	231	0.50D+01	0.00D+00	0.0
108	8	231	0.00D+00	0.00D+00	0.0
109	8	231	-0.60D+01	0.00D+00	0.0
110	8	231	-0.12D+02	0.00D+00	0.0
111	8	231	0.60D+02	0.00D+00	0.0
112	8	231	0.45D+02	0.00D+00	0.0
113	8	231	0.30D+02	0.00D+00	0.0
114	8	231	0.25D+02	0.00D+00	0.0
115	8	231	0.20D+02	0.00D+00	0.0

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

116	8	231	0.15D+02	0.00D+00	0.0
117	8	231	0.10D+02	0.00D+00	0.0
118	8	231	0.50D+01	0.00D+00	0.0
119	8	231	0.00D+00	0.00D+00	0.0
120	8	231	-0.60D+01	0.00D+00	0.0
121	8	231	-0.12D+02	0.00D+00	0.0
122	8	231	0.60D+02	0.00D+00	0.0
123	8	231	0.45D+02	0.00D+00	0.0
124	8	231	0.30D+02	0.00D+00	0.0
125	8	231	0.25D+02	0.00D+00	0.0
126	8	231	0.20D+02	0.00D+00	0.0
127	8	231	0.15D+02	0.00D+00	0.0
128	8	231	0.10D+02	0.00D+00	0.0
129	8	231	0.50D+01	0.00D+00	0.0
130	8	231	0.00D+00	0.00D+00	0.0
131	8	231	-0.60D+01	0.00D+00	0.0
132	8	231	-0.12D+02	0.00D+00	0.0
133	8	231	0.60D+02	0.00D+00	0.0
134	8	231	0.45D+02	0.00D+00	0.0
135	8	231	0.30D+02	0.00D+00	0.0
136	8	231	0.25D+02	0.00D+00	0.0
137	8	231	0.20D+02	0.00D+00	0.0
138	8	231	0.15D+02	0.00D+00	0.0
139	8	231	0.10D+02	0.00D+00	0.0
140	8	231	0.50D+01	0.00D+00	0.0
141	8	231	0.00D+00	0.00D+00	0.0
142	8	231	-0.60D+01	0.00D+00	0.0
143	8	231	-0.12D+02	0.00D+00	0.0
144	8	231	0.60D+02	0.00D+00	0.0
145	8	231	0.45D+02	0.00D+00	0.0
146	8	231	0.30D+02	0.00D+00	0.0
147	8	231	0.25D+02	0.00D+00	0.0
148	8	231	0.20D+02	0.00D+00	0.0
149	8	231	0.15D+02	0.00D+00	0.0
150	8	231	0.10D+02	0.00D+00	0.0
151	8	231	0.50D+01	0.00D+00	0.0
152	8	231	0.00D+00	0.00D+00	0.0
153	8	231	-0.60D+01	0.00D+00	0.0
154	8	231	-0.12D+02	0.00D+00	0.0
155	8	231	0.60D+02	0.00D+00	0.0
156	8	231	0.45D+02	0.00D+00	0.0
157	8	231	0.30D+02	0.00D+00	0.0
158	8	231	0.25D+02	0.00D+00	0.0
159	8	231	0.20D+02	0.00D+00	0.0
160	8	231	0.15D+02	0.00D+00	0.0
161	8	231	0.10D+02	0.00D+00	0.0
162	8	231	0.50D+01	0.00D+00	0.0
163	8	231	0.00D+00	0.00D+00	0.0
164	8	231	-0.60D+01	0.00D+00	0.0
165	8	231	-0.12D+02	0.00D+00	0.0

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

166	8	231	0.60D+02	0.00D+00	0.0
167	8	231	0.45D+02	0.00D+00	0.0
168	8	231	0.30D+02	0.00D+00	0.0
169	8	231	0.25D+02	0.00D+00	0.0
170	8	231	0.20D+02	0.00D+00	0.0
171	8	231	0.15D+02	0.00D+00	0.0
172	8	231	0.10D+02	0.00D+00	0.0
173	8	231	0.50D+01	0.00D+00	0.0
174	8	231	0.00D+00	0.00D+00	0.0
175	8	231	-0.60D+01	0.00D+00	0.0
176	8	231	-0.12D+02	0.00D+00	0.0
177	8	231	0.60D+02	0.00D+00	0.0
178	8	231	0.45D+02	0.00D+00	0.0
179	8	231	0.30D+02	0.00D+00	0.0
180	8	231	0.25D+02	0.00D+00	0.0
181	8	231	0.20D+02	0.00D+00	0.0
182	8	231	0.15D+02	0.00D+00	0.0
183	8	231	0.10D+02	0.00D+00	0.0
184	8	231	0.50D+01	0.00D+00	0.0
185	8	231	0.00D+00	0.00D+00	0.0
186	8	231	-0.60D+01	0.00D+00	0.0
187	8	231	-0.12D+02	0.00D+00	0.0
188	8	231	0.60D+02	0.00D+00	0.0
189	8	231	0.45D+02	0.00D+00	0.0
190	8	231	0.30D+02	0.00D+00	0.0
191	8	231	0.25D+02	0.00D+00	0.0
192	8	231	0.20D+02	0.00D+00	0.0
193	8	231	0.15D+02	0.00D+00	0.0
194	8	231	0.10D+02	0.00D+00	0.0
195	8	231	0.50D+01	0.00D+00	0.0
196	8	231	0.00D+00	0.00D+00	0.0
197	8	231	-0.60D+01	0.00D+00	0.0
198	8	231	-0.12D+02	0.00D+00	0.0
199	8	231	0.60D+02	0.00D+00	0.0
200	8	231	0.45D+02	0.00D+00	0.0
201	8	231	0.30D+02	0.00D+00	0.0
202	8	231	0.25D+02	0.00D+00	0.0
203	8	231	0.20D+02	0.00D+00	0.0
204	8	231	0.15D+02	0.00D+00	0.0
205	8	231	0.10D+02	0.00D+00	0.0
206	8	231	0.50D+01	0.00D+00	0.0
207	8	231	0.00D+00	0.00D+00	0.0
208	8	231	-0.60D+01	0.00D+00	0.0
209	8	231	-0.12D+02	0.00D+00	0.0
210	8	231	0.60D+02	0.00D+00	0.0
211	8	231	0.45D+02	0.00D+00	0.0
212	8	231	0.30D+02	0.00D+00	0.0
213	8	231	0.25D+02	0.00D+00	0.0
214	8	231	0.20D+02	0.00D+00	0.0
215	8	231	0.15D+02	0.00D+00	0.0

TABLE 6-3. INPUT DATA SET FOR THE THREE-DIMENSIONAL 3DFEMWATER PROBLEM (continued)

```
   216      8      231        0.10D+02        0.00D+00        0.0
   217      8      231        0.50D+01        0.00D+00        0.0
   218      8      231        0.00D+00        0.00D+00        0.0
   219      8      231       -0.60D+01        0.00D+00        0.0
   220      8      231       -0.12D+02        0.00D+00        0.0
   221      8      231        0.60D+02        0.00D+00        0.0
   222      8      231        0.45D+02        0.00D+00        0.0
   223      8      231        0.30D+02        0.00D+00        0.0
   224      8      231        0.25D+02        0.00D+00        0.0
   225      8      231        0.20D+02        0.00D+00        0.0
   226      8      231        0.15D+02        0.00D+00        0.0
   227      8      231        0.10D+02        0.00D+00        0.0
   228      8      231        0.50D+01        0.00D+00        0.0
   229      8      231        0.00D+00        0.00D+00        0.0
   230      8      231       -0.60D+01        0.00D+00        0.0
   231      8      231       -0.12D+02        0.00D+00        0.0
            0      0    0     0.0              0.0             0.0    END OF IC
C ******* DATA SET 12: SOURCE/SINK AND B. C. CONTROL INTEGERS
  0      0      0      0      0      0      0      0     165      2      2      0
  0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
C ******* DATA SET 15: DIRICHLET BOUNDARY CONDITIONS
   0.0D0    60.0D0     1.0D38     60.0D0
   0.0D0    30.0D0     1.0D38     30.0D0

    1    2    3    4    5    6    7    8    9  232  233  234  235  236  237  238
  239  240  463  464  465  466  467  468  469  470  471  694  695  696  697  698
  699  700  701  702  925  926  927  928  929  930  931  932  933 1156 1157 1158
 1159 1160 1161 1162 1163 1164 1387 1388 1389 1390 1391 1392 1393 1394 1395 1618
 1619 1620 1621 1622 1623 1624 1625 1626 1849 1850 1851 1852 1853 1854 1855 1856
 1857  221  222  223  224  225  226  227  228  229  452  453  454  455  456  457
  458  459  460  683  684  685  686  687  688  689  690  691  914  915  916  917
  918  919  920  921  922 1145 1146 1147 1148 1149 1150 1151 1152 1153 1376 1377
 1378 1379 1380 1381 1382 1383 1384 1607 1608 1609 1610 1611 1612 1613 1614 1615
 1838 1839 1840 1841 1842 1843 1844 1845 1846 2069 2070 2071 2072 2073 2074 2075
 2076 2077  111  112  113
    1  161    1    1    0
  163    2    1    2    0
    0    0    0    0    0  END OF IDTYP
    0    END OF JOB  ----------------------------------------------------------------000
```

6.2 3DLEWASTE

To demonstrate the application of 3DLEWASTE, two simple example problems are presented. For each problem, a brief description and a correctly-constructed input data set are given. The corresponding output is not included in this documentation. Rather, it is distributed along with the code by the EPA Center for Exposure Assessment Modeling (CEAM) at the Environmental Research Laboratory in Athens, Georgia. See Section 2 for information about obtaining the code.

6.2.1 One-Dimensional Transport Problem

Transient one-dimensional transport through a horizontal column is simulated in this example (Figure 6.4). The dimensions of the column are identical to those of the column in Figure 6.1. It has a length of 200 cm and a 50 cm x 50 cm cross-section. Initially, the concentration is 0.0 g/cm^3 throughout the region of interest. The concentration at x = 0.0 cm is maintained at C = CO = 1.0 g/cm^3 (a Dirichlet boundary). A variable boundary condition is used to specify the natural condition of zero gradient flux at x = 200.0 cm. A bulk density of 1.2 g/cm^3 and a longitudinal dispersivity of 5.0 cm are assumed. No adsorption or decay is allowed. A specific discharge (Darcy velocity) of 2.0 cm/d is assumed and a moisture content of 0.4 is used.

The region of interest, that is, the whole column, is discretized with 1 x 1 x 40 = 40 elements with the element size equal to 50 x 50 x 5 cm. This results in 2 x 2 x 41 = 164 node points. For this simulation, each of the four vertical lines is considered a subregion. Thus, a total of four subregions, each with 41 node points, is used for the subregional block iteration simulation. A constant time-step size of 0.5 is used and a 40 time-step simulation is run. For this discretization, the mesh Peclet number is P_e = 1 and the Courant number is C_r = 0.5.

The input data set for this problem, prepared according to the instructions in Sections 4.2 and 5.2, is shown in Table 6-4.

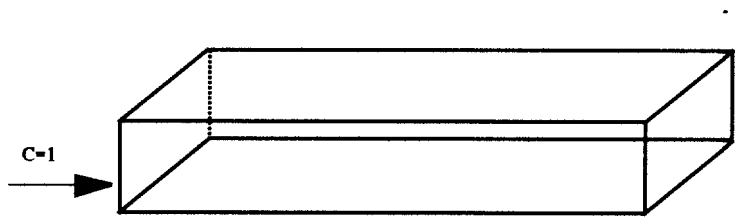

Figure 6.4. One-dimensional transient transport through a horizontal column.

TABLE 6-4. INPUT DATA SET FOR THE ONE-DIMENSIONAL 3DLEWASTE PROBLEM

```
 1 ONE-D FIRST TYPE BOUNDARY VALUE PROBLEM WITH 3DLEWASTE L=CM,T=DAY,M=G 00
C ******* DATA SET 2: BASIC INTEGER PARAMETERS ***** **************************
 164  40   1   0   40   1   8  -1   1   0   1   1   1  100   1
C ******* DATA SET 3: BASIC REAL PARAMETERS ***** ******************************
  0.50D0  0.0D0  1.0D0  20.0D0  1.0D00  1.0D0  1.0D-3  1.0D-4
C ******* DATA SET 4: PRINTER, STORAGE AND TIME RESETTING CONTROL *************
55000000005000000000500000000050000000005
11000000001000000000100000000010000000001
  1.0D38
C ******* DATA SET 5: MATERIAL PROPERTIES ***********************************
  0.0D0  1.2D0  5.0D0  0.0D0  0.0D0  1.0D0  0.0D0  0.0D0
C **** *** DATA SET 6: NODE COORDINATES ***************************************
  1 40 1 0.0D0 50.0D0 0.0D0 0.0D0 0.0D0 5.0D0
 42 40 1 0.0D0 0.0D0 0.0D0 0.0D0 0.0D0 5.0D0
 83 40 1 50.0D0 0.0D0 0.0D0 0.0D0 0.0D0 5.0D0
124 40 1 50.0D0 50.0D0 0.0D0 0.0D0 0.0D0 5.0D0
   0 0 0      0.0      0.0      0.0      0.0    0.0    0.0      END OF COORDINATES
C ******* DATA SET 7: ELEMENT CONNECTIVITY ***** *******************************
  1 39  1 42 83 124  1 43 84 125 2  1
  0 0  0   0   0 0   0   0   0   0 0 0       END OF IE
C ******* DATA SET 8: SUBREGIONAL DATA ***** ************************************
    4
  1  3  1  41  0
  0 0 0 0 0                              END OF NNPLR(K)
  1 40  1  1  1
  0 0 0 0 0                              END OF GNLR(I,1)
  1 40  1 42  1
  0 0 0 0 0                              END OF GNLR(I,2)
  1 40  1 83 1
 0 0 0 0 0                               END OF GNLR(I,3)
    1   40    1  124    1
 0 0 0 0 0                               END OF GNLR(I,4)
C ******* DATA SET 10: INITIAL CONDITIONS ***** ********************************
     1      3      41         1.0D0     0.0D0     0.0
     2     38       1         0.0D0     0.0D0     0.0
    43     38       1          .0D0     0.0D0     0.0
    84     38       1         0.0D0     0.0D0     0.0
   125     38       1         0.0D0     0.0D0     0.0
    41      3      41         0.0D0     0.0D0     0.0
    0  0  0  0.0  0.0  0.0                          END OF IC
C ******* DATA SET 11: SOURCE/SINK AND B. C. CONTROL INTEGERS ***** ************
 0 0 0 0  0 0 0 0  4 1 2 0
 1 4 1 2 0  0 0 0 0 0  0 0 0 0 0
```

TABLE 6-4. INPUT DATA SET FOR THE ONE-DIMENSIONAL 3DLEWASTE PROBLEM (concluded)

```
C ******* DATA SET 13: VARIABLE BOUNDARY CONDITIONS ***** **********************
 0.0D0  0.0D0  1.0D38  0.0D0
   1    0    0    1    0
   0    0    0    0    0                  END OF IRTYP
   1  0  0  82 123 164 41 0 0 0 0
   0  0  0   0   0   0  0 0 0 0 0 0          END OF ISV(J,I) J=1,4
   1    3    1   41   41
   0    0    0    0    0                  END OF NPVB
C ******* DATA SET 14: DIRICHLET BOUNDARY CONDITIONS **************************
    0.0D0     1.0D0    1.0D38     1.0D0
   1   42   83   124
   1    3    1    1    0
   0    0    0    0    0                  END OF IDTYP
C ******* DATA SET 16: HYDROLOGICAL BOUNDARY CONDITIONS ************************
 1 163 1 0.0D0 0.0D0 2.0D0 0.0D0 0.0D0 0.0D0
 0  0 0  0.0  0.0  0.0  0.0  0.0  0.0  END  OF  VELOCITY
   1  39  1  0.4D0  0.0
   0    0    0    0.0    0.0              END OF TH
   0 ***************** END OF JOB ***** ****************************************00
```

6.2.2 Two-Dimensional Transport in a Rectangular Region

This is a two-dimensional transport problem in a rectangular region 600.0 cm long, 270.0 cm high, and 1.0 cm thick (Figure 6.5). Initially, the concentration is zero g/cm^3 throughout the region of interest. A concentration of 1.0 g/cm^3 is maintained at x = 0.0 cm and 180.0 cm < y <270.0 cm by applying a Dirichlet boundary condition. A concentration of 0.0 g/cm^3 is maintained at x = 0.0 cm and 0.0 cm < y < 90.0 cm and 180.0 cm < y <270.0 cm. A natural condition is imposed at x = 600 cm using a variable boundary condition (Equation 3-39b). A single material with a bulk density of 1.2 g/cm^3, a longitudinal dispersivity of 10.0 cm, and a lateral dispersivity of 1.0 cm modeled. No adsorption or decay is allowed. A specific discharge (Darcy velocity) of 2.0 cm/d is used and a moisture content of 0.2 is assumed.

The region is divided into 9 x 9 x 1 = 81 elements, resulting in 10 x 10 x 2 = 200 nodes. The element size is 60.0 cm x 30.0 cm x 1.0 cm. Each of the two vertical planes is considered a subregion. Thus, a total of two subregions, each with 100 nodal points, is used for the subregional block iteration simulation. A time-step size of 4.5 is used and 40 time steps are simulated.

The input data set for this problem, prepared according to the instructions in Sections 4.2 and 5.2, is shown in Table 6-5.

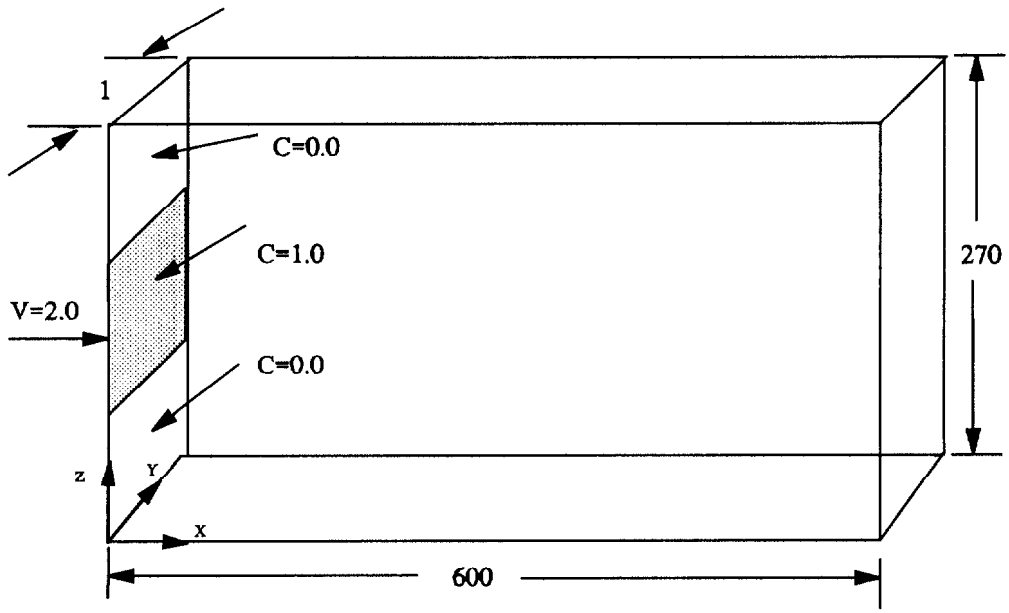

Figure 6.5. Two-dimensional transient transport in a rectangular region.

TABLE 6-5. INPUT DATA SET FOR THE TWO-DIMENSIONAL 3DLEWASTE PROBLEM

```
1 TWO-D FIRST TYPE BOUNDARY VALUE PROBLEM WITH 3DLEWASTE L=CM,T=DAY,M=G 00
C ******* DATA SET 2: BASIC INTEGER PARAMETERS ***** **************************
 200 81 1 0 40 1 8  -1  1  0  1  1  1   200  1
C ******* DATA SET 3: BASIC REAL PARAMETERS ***** ******************************
  0.45D1 0.0D0 9.0D0 3.60D2 1.0D00 1.78D0 1.0D-3 1.0D-4
C ******* DATA SET 4: PRINTER, STORAGE AND TIME RESETTING CONTROL *************
55000000005000000000500000000050000000005
11000000001000000000100000000010000000001
   1.0D38
C **** *** DATA SET 5: MATERIAL PROPERTIES ************************************
  0.0D0 1.2D0 10.0D0 1.0D0 0.0D0 1.0D0 0.0D0 0.0D0
C **** *** DATA SET 6: NODE COORDINATES ***************************************
    1    9   10   0.0D0     0.0D0    0.0D0    6.0D1    0.0D0    0.0D0
    2    9   10   0.0D0     3.0D1    0.0D0    6.0D1    0.0D0    0.0D0
    3    9   10   0.0D0     6.0D1    0.0D0    6.0D1    0.0D0    0.0D0
    4    9   10   0.0D0     9.0D1    0.0D0    6.0D1    0.0D0    0.0D0
    5    9   10   0.0D0    12.0D1    0.0D0    6.0D1    0.0D0    0.0D0
    6    9   10   0.0D0    15.0D1    0.0D0    6.0D1    0.0D0    0.0D0
    7    9   10   0.0D0    18.0D1    0.0D0    6.0D1    0.0D0    0.0D0
    8    9   10   0.0D0    21.0D1    0.0D0    6.0D1    0.0D0    0.0D0
    9    9   10   0.0D0    24.0D1    0.0D0    6.0D1    0.0D0    0.0D0
   10    9   10   0.0D0    27.0D1    0.0D0    6.0D1    0.0D0    0.0D0
  101    9   10   0.0D0     0.0D0    1.0D0    6.0D1    0.0D0    0.0D0
  102    9   10   0.0D0     3.0D1    1.0D0    6.0D1    0.0D0    0.0D0
  103    9   10   0.0D0     6.0D1    1.0D0    6.0D1    0.0D0    0.0D0
  104    9   10   0.0D0     9.0D1    1.0D0    6.0D1    0.0D0    0.0D0
  105    9   10   0.0D0    12.0D1    1.0D0    6.0D1    0.0D0    0.0D0
  106    9   10   0.0D0    15.0D1    1.0D0    6.0D1    0.0D0    0.0D0
  107    9   10   0.0D0    18.0D1    1.0D0    6.0D1    0.0D0    0.0D0
  108    9   10   0.0D0    21.0D1    1.0D0    6.0D1    0.0D0    0.0D0
  109    9   10   0.0D0    24.0D1    1.0D0    6.0D1    0.0D0    0.0D0
  110    9   10   0.0D0    27.0D1    1.0D0    6.0D1    0.0D0    0.0D0
 0  0  0       0.0         0.0          0.0      0.0      0.0      0.0       END OF COORDINATES
C ******* DATA SET 7: ELEMENT CONNECTIVITY ***** *******************************
    1  8   1    1   11   12    2  101  111  112  102  1
   10  8   1   11   21   22   12  111  121  122  112  1
   19  8   1   21   31   32   22  121  131  132  122  1
   28  8   1   31   41   42   32  131  141  142  132  1
   37  8   1   41   51   52   42  141  151  152  142  1
   46  8   1   51   61   62   52  151  161  162  152  1
   55  8   1   61   71   72   62  161  171  172  162  1
   64  8   1   71   81   82   72  171  181  182  172  1
   73  8   1   81   91   92   82  181  191  192  182  1
   0 0   0    0    0    0    0    0    0    0   0   0          END OF IE
C ******* DATA SET 8: SUBREGIONAL DATA ***** ***********************************
    2
  1   1   1  100  0
  0  0  0  0  0                              END OF NNPLR(K)
  1  99  1   1   1
  0  0  0  0  0                              END OF GNLR(I,1)
  1  99  1  101  1
  0  0  0  0  0                              END OF GNLR(I,2)
```

TABLE 6-5. INPUT DATA SET FOR THE TWO-DIMENSIONAL 3DLEWASTE PROBLEM (concluded)

```
C ******* DATA SET 10: INITIAL CONDITIONS ************************************
   1  199  1        0.0D0    0.0D0  0.0
   0  0  0  0.0  0.0  0.0                    END OF IC
C ******* DATA SET 11: SOURCE/SINK AND B. C. CONTROL INTEGERS *****************
 0   0  0  0  0  0  0  0  8  1  2  0
 9  10  1  2  0  0  0  0  0  0  0  0  0  0  0
C *** **** DATA SET 13: VARIABLE BOUNDARY CONDITIONS ***************************
  0. 0D0 0.0D0 1.0D38 0.0D0
   1    8    1    1    0
   0    0    0    0    0                          END OF IRTYP
   1  8  1  91  92  192  191  1  1  1  1
   0  0  0   0   0   0  0   0    0    0   0        END OF ISV(J,I) J=1,4
   1    9    1   91    1
   0    0    0    0    0                          END OF NPVB
C ******* DATA SET 14: DIRICHLET BOUNDARY CONDITIONS ***************************
    0.0D0    1.0D0   1.0D38    1.0D0
   4   5   6   7   104   105   106   107
   1    7    1    1    0
   0    0    0    0    0                          END OF IDTYP
C ******* DATA SET 16: HYDROLOGICAL BOUNDARY CONDITIONS ************************
 1  199  1  2.0D0  0.0D0  0.0D0  0.0D0  0.0D0  0.0D0
 0   0  0    0.0    0.0    0.0    0.0    0.0    0.0      END OF VELOCITY
   1   80    1  0.2D0  0.0
   0    0    0    0.0    0.0                        END OF TH
   0**************** END OF JOB ********** ***** ***** ***** ***** **********00
```

SECTION 7

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APPENDIX A

PROGRAM STRUCTURE AND SUBROUTINE DESCRIPTIONS

A.1 3DFEMWATER

3DFEMWATER consists of a main program, FEMWAT3D, and 22 subroutines. Figure A. 1 shows the structure of the program. The subroutines are listed in Table A-1 and the functions of these subroutines are briefly described below.

A. 1.1 Subroutine ALLFCT

This subroutine is called by subroutine GW3D to compute values for all the source/sink and boundary nodes and elements. It uses linear interpolation of tabular data to simulate variations in time for these conditions.

A.1.2 Subroutine ASEMBL

This subroutine is called by subroutine GW3D. After calling subroutine Q8 to evaluate the element matrices, it sums over all element matrices to form a global matrix equation governing the pressure head at all nodes.

A. 1.3 Subroutine BASE

This subroutine is called by subroutines Q8DV and Q8 to evaluate the value of the base function at a Gaussian point.

A. 1.4 Subroutine BC

This subroutine, which is called by subroutine GW3D, incorporates Dirichlet, variable composite, specified-flux (Cauchy), and specified-pressure-head gradient (Neumann) boundary conditions. For a Dirichlet boundary condition, an identity algebraic equation is generated for each Dirichlet nodal point. Any other equation having this nodal variable is modified accordingly to simplify the computation. For a specified-flux surface, the integration of the surface source is obtained by calling subroutine Q4S and the result is added to the load vector. For a specified-pressure-head gradient surface, the integrations of both the gradient and gravity fluxes are obtained by calling the subroutine Q4S. These fluxes are added to the load vector. The subroutine BC also implements the variable composite boundary condition. First, it checks all infiltration-evapotranspiration-seepage points, identifying any of them that are Dirichlet

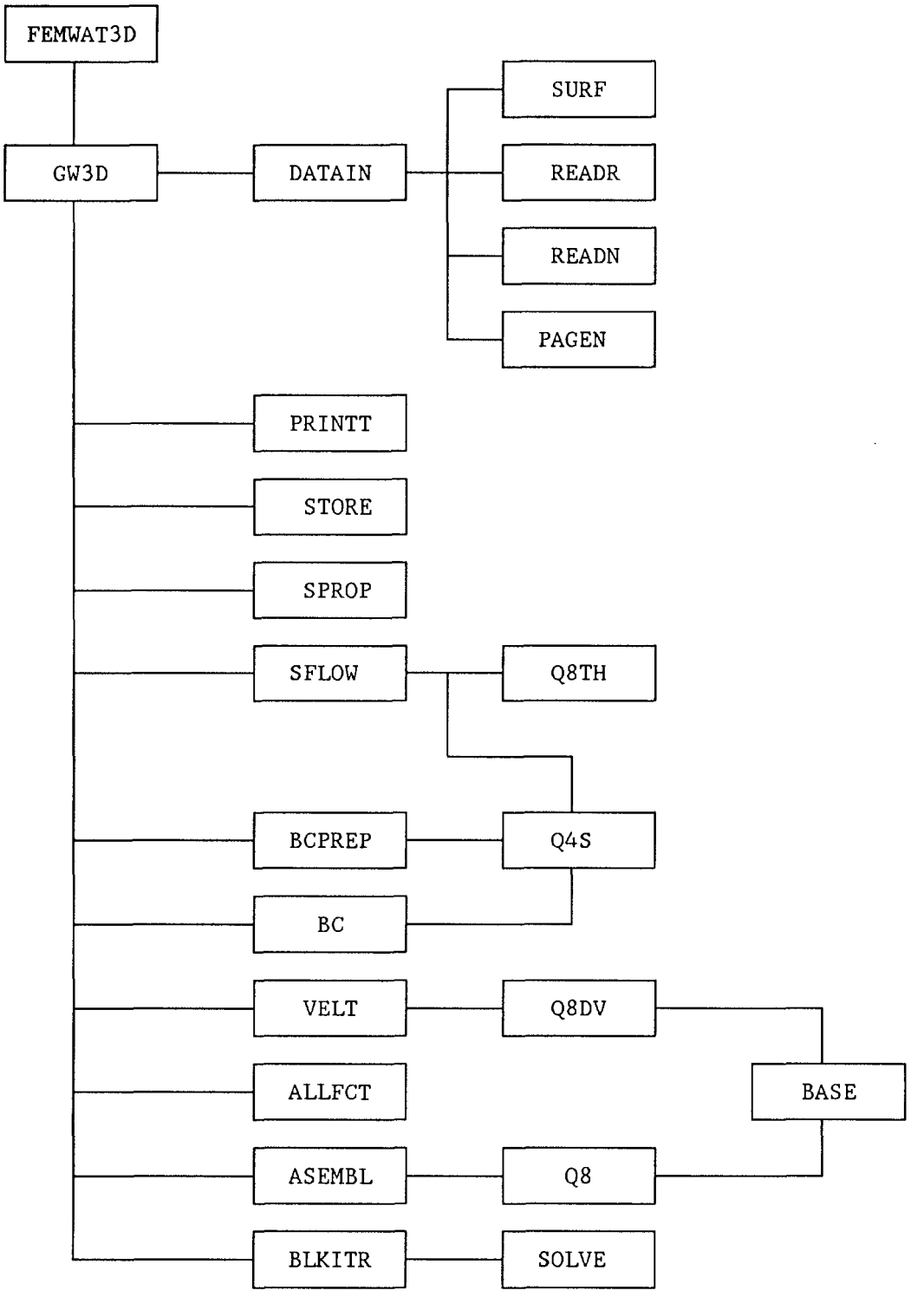

Figure A. 1. Program structure of 3DFEMWATER

TABLE A-1. SUBROUTINES INCLUDED IN 3DFEMWATER

Subroutine	Called By	Description
ALLFCT	GW3D	Interpolates functional values for source/sink and boundary conditions.
ASEMBL	GW3D	Evaluates the element matrices and then sums over all element matrices to form a global matrix equation governing the pressure head at all nodes.
BASE	Q8DV, Q8	Evaluates the value of the base function at a Gaussian point.
BC	GW3D	Incorporates Dirichlet, specified-flux (Cauchy), specified-pressure-head gradient (Neumann), and variable composite boundary conditions.
BCPREP	GW3D	Prepares the infiltration/seepage boundary conditions during a rainfall period or the seepage/evapotranspiration boundary conditions during non-rainfall periods.
BLKITR	GW3D	Solves the matrix equation with block iteration methods.
DATAIN	GW3D	Reads and prints all input information.
GW3D	FEMWAT3D	Controls the entire sequence of operations. Performs either the steady-state computation alone, or a transient-state computation using the steady-state solution as the initial condition, or a transient computation using user-supplied initial conditions.
PAGEN	DATAIN	Preprocesses pointer arrays that are needed to store the global matrix in compressed form and to construct the subregional block matrices.
PRINTT	GW3D	Prints the flow variables, which include the fluxes through variable boundary surfaces, pressure head, total head, moisture content, and Darcy velocity components.

TABLE A-1. SUBROUTINES INCLUDED IN 3DFEMWATER (continued)

Subroutine	Called By	Description
Q4S	BCPREP, BC,	Evaluates the boundary surface load vector SFLOW over a SFLOW boundary segment.
Q8	ASEMBL	Computes the element matrices and element load vector.
Q8DV	VELT	Computes the integration of N(I)*N(J) and -N(I)* K42RAD(HT) over an element.
Q8TH	SFLOW	Evaluates the integration of moisture content and sources/sinks over an element.
READN	DATAIN	Automatically generates integer input if required.
READR	DATAIN	Automatically generates real number input if required.
SFLOW	GW3D	Computes the fluxes through boundaries and the rate at which water content increases in the region of interest.
SOLVE	BLKITR	Solves a matrix equation with the direct band method.
SPROP	GW3D	Calculates the values of moisture content, relative hydraulic conductivity, and water capacity using van Genuchten analytical functions.
STORE	GW3D	Stores the solution in binary on logical unit LUSTO. Information stored includes regional geometry, subregion data, and hydrological variables such as pressure head, total head, moisture content, and the Darcy velocity components.
SURF	DATAIN	Identifies the boundary sides, sequences the boundary nodes, and computes the direction-al cosine of the surface sides.

TABLE A-1. SUBROUTINES INCLUDED IN 3DFEMWATER (continued)

Subroutine	Called By	Description
VELT	GW3D	Evaluates the element matrices and the derivatives of the total head, and then sums over all element matrices to form a matrix equation governing the velocity components at all nodal points.

points. If there are Dirichlet points, they are incorporated using the method described above. If a given point is not a Dirichlet point, the point is bypassed. Second, it checks all rainfall-evaporation-seepage points again to see if any of them is a specified-flux point. If it is, then the computed flux by infiltration or potential evapotranspiration is added to the load vector. If a given point is not a specified-flux point, it is bypassed. Because the infiltration-evaporation-seepage points are either Dirichlet or specified-flux points, all points are taken care of in this manner.

A. 1.5 Subroutine BCPREP

This subroutine is called by GW3D to prepare the infiltration-seepage boundary conditions during a rainfall period or the seepage-evapotranspiration boundary conditions during non-rainfall periods. It decides the number of nodal points on the variable boundary to be considered as Dirichlet or specified-flux (Cauchy) points. It computes the number of points that change boundary conditions from 1) ponding depth (Dirichlet types) to infiltration (specified-flux types), or 2) infiltration to pending depth, or 3) minimum pressure (Dirichlet types) to infiltration during rainfall periods. It also computes the number of points that change boundary conditions from potential evapotranspiration (specified-flux types) to minimum pressure, or from ponding depth to potential evapotranspiration, or from minimum pressure to potential evapotranspiration during non-rainfall periods. Upon completion, this subroutine returns the Darcy flux (DCYFLX), infiltration/potential evapotranspiration rate (FLX), the ponding depth nodal index (NPCON), the flux-type nodal index (NPFI.X), the minimum pressure nodal index (NPMIN), and the number of nodal points (NCHG) that have changed boundary conditions.

A.1.6 Subroutine BLKITR

This subroutine is called by subroutine GW3D to solve the matrix equation with block iteration methods. For each subregion, a block matrix equation is constructed based on the global matrix equation and two pointer arrays, GNPLR and LNOJCN (see subroutine PAGEN), and the resulting block matrix equation is solved with the direct band matrix solver by calling subroutine SOLVE. This is done for all subregions for each iteration until a convergent solution is obtained.

A.1.7 Subroutine DATAIN

Subroutine DATAIN is called by subroutine GW3D. It reads all data input described in Section 4.1 except data set 1. It also calls subroutine SURF to identify the surface elements and boundary nodes, and subroutines READR and READN, respectively, to automatically generate real and integer numbers.

A.1.8 Subroutine GW3D

Subroutine GW3D controls the entire sequence of operations. It performs either a steady-state computation alone (KSS = 0 and NTI = 0), or a transient- state computation using the steady-state solution as the initial condition (KSS = 0, NTI > 0), or a transient computation using user-supplied initial conditions (KSS = 1, NTI > 0).

GW3D calls subroutine DATAIN to read and print input data; subroutine PAGEN to generate pointer arrays; subroutine ALLFCT to obtain source/sink and boundary values; subroutine SPROP to obtain the relative hydraulic conductivity, water capacity, and moisture content from the pressure head; subroutine VELT to compute Darcy velocity, subroutine BCPREP to determine if a change of boundary conditions is required, subroutine ASEMBL to assemble the element matrices over all elements; subroutine BC to implement the boundary conditions; subroutine BLKITR to form and solve the subregional block matrix equations; subroutine SFLOW to calculate flux through all types of boundaries and water accumulated in the media; subroutine PRINTT to print out the results; and subroutine STORE to store the flow variables for input to 3DLEWASTE or for plotting.

A. 1.9 Subroutine PAGEN

This subroutine is called by subroutine DATIUN to preprocess pointer arrays that are needed to store the global matrix in compressed form and to construct the subregional block matrices. The pointer arrays automatically generated in this subroutine include the global node connectivity (stencil), GNOJCN(J,N), regional node connectivity, LNOJCN(J,I,K), total node number for each subregion, NTNPLR(K), the bandwidth indicator for each subregion, LMAXDF(K), and a partial fall-up for the mapping array between global node number and local subregion node number, GNPLR(I,K), with I = NNPLR(K) + 1 to NTNPLR(K). Here GNOJCN(J,N) is the global node number of the J-th node connected to the global node N; LNOJCN(J,I,K) is the local node number of the J-th node connected to the local node I in the K-th subregion; NTNPLR(K) is the total number of nodes in the K-th subregion, including the interior nodes, the global boundary nodes, and intra-boundary nodes; LMAXDF(K) is the maximum difference between any two nodes of any element in the K-th subregion; and GNPLR(I,K) is the global node number of the I-th local-region node in the K-th subregion. These pointer arrays are generated based on the element connectivity, IE(M,J), the number of nodes for each subregion, NNPLR(K), and the mapping between global node and local-region node, GNLR(I,K), with I = 1, NNPLR(K). Here IE(M,J) is the global node number of J-th node of element M; NNPLR(K) is the number of nodes in the K-th subregion, including the interior nodes and the global boundary nodes, but not the intraboundary nodes.

A. 1.10 Subroutine PRINTT

This subroutine, which is called by GW3D, is used to line-print the flow variables. These include the fluxes through variable boundary surfaces, the pressure head, total head, moisture content, and Darcy velocity components.

A. 1.11 Subroutine Q4S

This subroutine is called by subroutines BC, BCPREP, and SFLOW to compute the surface node flux of the type:

$$RQ(I) = \int_{B_e} N_i^e q \, dB \tag{A-1}$$

where q is either the specified-flux, specified-pressure-head gradient flux, or gravity flux; B is the global boundary of the region of interest; N_i^e is the basis functions for nodal point i of element e; and RQ(I) is a 3DFEMWATER code parameter.

A.1.12 Subroutine Q8

This subroutine is called by the subroutine ASEMBL to compute the element matrix given by

$$QA(I,J) = \int_{R_e} N_i^e F \, N_j^e \, d\,R \tag{A-2a}$$

$$QB(I,J) = \int_{R_e} (\nabla N_i^e) \cdot \mathbf{K}_s k_r (\nabla N_j^e) dR \tag{A-2b}$$

where

F	=	soil property function
N_j^e	=	basis function for nodal point j of element e
$\mathbf{K}_s$	=	saturated hydraulic conductivity tensor
k_r	=	relative hydraulic conductivity
R	=	region of interest
∇	=	del operator indicating gradient
$\nabla\cdot$	=	del operator indicating divergence

and where QA(I,J) and QB(I,J) are 3DFEMWATER code parameters. Subroutine Q8 also calculates the element load vector given by:

$$RQ(I) = \int_{R_e} [(\nabla N_i^e) \cdot \mathbf{K}_s k_r (\nabla z) - N_i^e q] dR \tag{A-2c}$$

where q is the source/sink.

A. 1.13 Subroutine Q8DV

Subroutine Q8DV is called by subroutine VELT to compute the element matrices given by:

$$QR(I,J) = \int_{R_e} N_i^e N_j^e dR \qquad \text{(A-3a)}$$

where QR(I,J) is a 3DFEMWATER program variable. Subroutine Q8DV also evaluates the element load vector:

$$QRX(I) = -\int_{R_e} N_i^e \mathbf{i} \cdot \mathbf{K}_s k_r (\nabla N_j^e) H_j dR \qquad \text{(A-3b)}$$

$$QRY(I) = -\int_{R_e} N_i^e \mathbf{j} \cdot \mathbf{K}_s k_r (\nabla N_j^e) H_j dR \qquad \text{(A-3c)}$$

$$QRZ(I) = -\int_{R_e} N_i^e \mathbf{k} \cdot \mathbf{K}_s k_r (\nabla N_j^e) H_j dR \qquad \text{(A-3d)}$$

where

H_j = total head at nodal point j
$\mathbf{i}$ = unit vector along the x-coordinate
$\mathbf{j}$ = unit vector along the y-coordinate
$\mathbf{k}$ = unit vector along the z-coordinate

and where QRX(I), QRY(I), and QRZ(I) are 3DFEMWATER program variables.

A. 1.14 Subroutine Q8TH

This subroutine, which is called by subroutine SFLOW, is used to compute the contribution from an element to the change in water content over time, using the following equation:

$$QTHP = \int_{R_e} \frac{d\theta}{dh} \frac{\partial h}{\partial t} dR \qquad \text{(A-4)}$$

where

h = pressure head
θ = moisture content
QTHP = 3DFEMWATER program variable

A.1.15 Subroutine READN

This subroutine is called by subroutine DATAIN to generate integer numbers for input data sets 8, 9, 12(c), 12(f), 14(b) through 14(d), 15(c), 16(b), 16(c), 17(b), and 17(c), which are described in Section 4.1.

A. 1.16 Subroutine READR

This subroutine is called by subroutine DATAIN to generate real numbers input for data sets 7, 14(e), and 14(f) (see Section 4.1). Automatic generation of regularly patterned data is built into this subroutine.

A. 1.17 Subroutine SFLOW

This subroutine is called by subroutine GW3D. It is used to compute the fluxes through various types of boundaries and the rate at which water content increases in the region of interest. In this subroutine, the function of variable FRATE(7) is to store the flux through the whole boundary enclosing the region of interest. It is given by:

$$\mathbf{FRATE(7)} = \int_{B}(V_x n_x + V_y n_y + V_z n_z)dB \qquad \text{(A-5)}$$

where V_x, V_y, and V_z are Darcy velocity components, and n_x, n_y, and n_z are the directional cosines of the outward unit vector normal to the boundary B. FRATE(l) through FRATE(5) store the flux through the Dirichlet boundary, B_D, specified-flux boundary, B_C, specified-pressure-head boundary, B_N, the seepage/evapotranspiration boundary, B_S, and infiltration boundary, B_R, respectively, and are given by:

$$\mathbf{FRATE(1)} = \int_{B_d}(V_x n_x + V_y n_y + V_z n_z)dB \qquad \text{(A-6a)}$$

$$\text{FRATE(2)} = \int_{B_c}(V_x n_x + V_y n_y + V_z n_z)dB \qquad \text{(A-6b)}$$

$$\mathbf{FRATE(3)} = \int_{B_n}(V_x n_x + V_y n_y + V_z n_z)dB \qquad \text{(A-6C)}$$

FRATE(6), which is related to the numerical loss, is given by:

$$FRATE(4) = \int_{B_x} (V_x n_x + V_y n_y + V_z n_z) dB \quad \text{(A-6d)}$$

$$FRATE(5) = \int_{B_z} (V_x n_x + V_y n_y + V_z n_z) dB \quad \text{(A-6e)}$$

$$FRATE(6) = FRATE(7) - \sum_{I=1}^{5} FRATE(I) \quad \text{(A-7)}$$

FRATE(8) and FRATE(9) are used to store the source/sink and increased rate of water accumulation within the media, respectively:

$$FRATE(8) = -\int_{R} q dR \quad \text{(A-8)}$$

and

$$FRATE(9) = \int_{R} F \frac{\partial h}{\partial t} dR \quad \text{(A-9)}$$

If there is no numerical error in the computation, the following equation should be satisfied:

$$FRATE(9) = -[FRATE(7) + FRATE(8)] \quad \text{(A-10)}$$

and FRATE(6) should be equal to zero.

A.1.18 Subroutine SOLVE

This subroutine is called by the subroutine BLKITR to solve a matrix equation of the type:

$$[c]\{x\} = \{y\} \quad \text{(A-11)}$$

where [C] is the coefficient matrix and {x) and {y) are two vectors. {x) is the unknown to be solved, and {y) is the known load vector. The computer returns the solution and stores it in {y). The computation is a standard banded Gaussian direct elimination procedure.

A. 1.19 Subroutine SPROP

This subroutine is called by subroutine GW3D. It calculates the values for moisture content, relative hydraulic conductivity, and water capacity, using the van Genuchten functional relationships (see Equations 3-3a through 3-3d).

A.1.20 Subroutine STORE

This subroutine, which is called by GW3D, is used to store the flow variables in a binary file. The stored data are intended for use in 3DLEWASTE or for plotting. The information stored includes region geometry, subregion data, and hydrological variables such as pressure head, total head, moisture content, and Darcy velocity components.

A. 1.21 Subroutine SURF

Subroutine SURF is called by subroutine DATAIN. It identifies the boundary sides, sequences the boundary nodes, and computes the directional cosine of the surface sides. The mappings from boundary nodes to global nodes are stored in NPBB(I) (where NPBB(I) is the global node number of the I-th boundary node). The boundary node numbers of the four nodes for each boundary side are stored in ISB(I,J) (where ISB(I,J) is the boundary node number of I-th node of J-th side, I = 1 to 4). There are six sides for each element. Which of these six sides is the boundary side is determined automatically in the subroutine SURF and is stored in ISB(5,J). The global element number, to which the J-th boundary side belongs, is also preprocessed in the subroutine SURF and is stored in ISB(6,J). The directional cosines of the J-th boundary side are computed and stored in DCOSB(I,J) (where DCOSB(I,J) is the directional cosine of the J-th surface with I-th coordinate, I = 1 to 3). The information contained in NPBB, ISB, and DOSB, along with the number of boundary nodes and the number of boundary sides, is returned to subroutine DATAIN for other uses.

A. 1.22 Subroutine VELT

This subroutine is called by subroutine GW3D. It calls subroutine Q8DV to evaluate the element matrices and the derivatives of the total head. It then sums over all element matrices to form a matrix equation governing the velocity components at all nodal points. To save computational time, the matrix is diagonalized by lumping. The velocity components can thus be solved point by point. The computed velocity field is then returned to GW3D through the argument. This velocity field is also passed to subroutine BCPREP to evaluate the Darcy flux across the seepage-infiltration-evapotranspiration surfaces.

A.2 3DLEWASTE

LEWASTE consists of a main program, LEWAST3D, 30 subroutines, and a function. Figure A.2 shows the structure of the program. The subroutines' and function are listed in Tables A-2 and A-3, respectively, and the purposes of the subroutines are briefly described below.

A.2.1 Subroutine ADVBC

This subroutine is called by GM3D to implement the boundary conditions. For a Dirichlet boundary, the Lagrangian concentration is specified. For variable boundaries, if the flow is directed out of the region, the fictitious particle associated with the boundary node must come from the interior nodes. Hence the Lagrangian concentration for the boundary node has already been computed from subroutine ADVTRN and

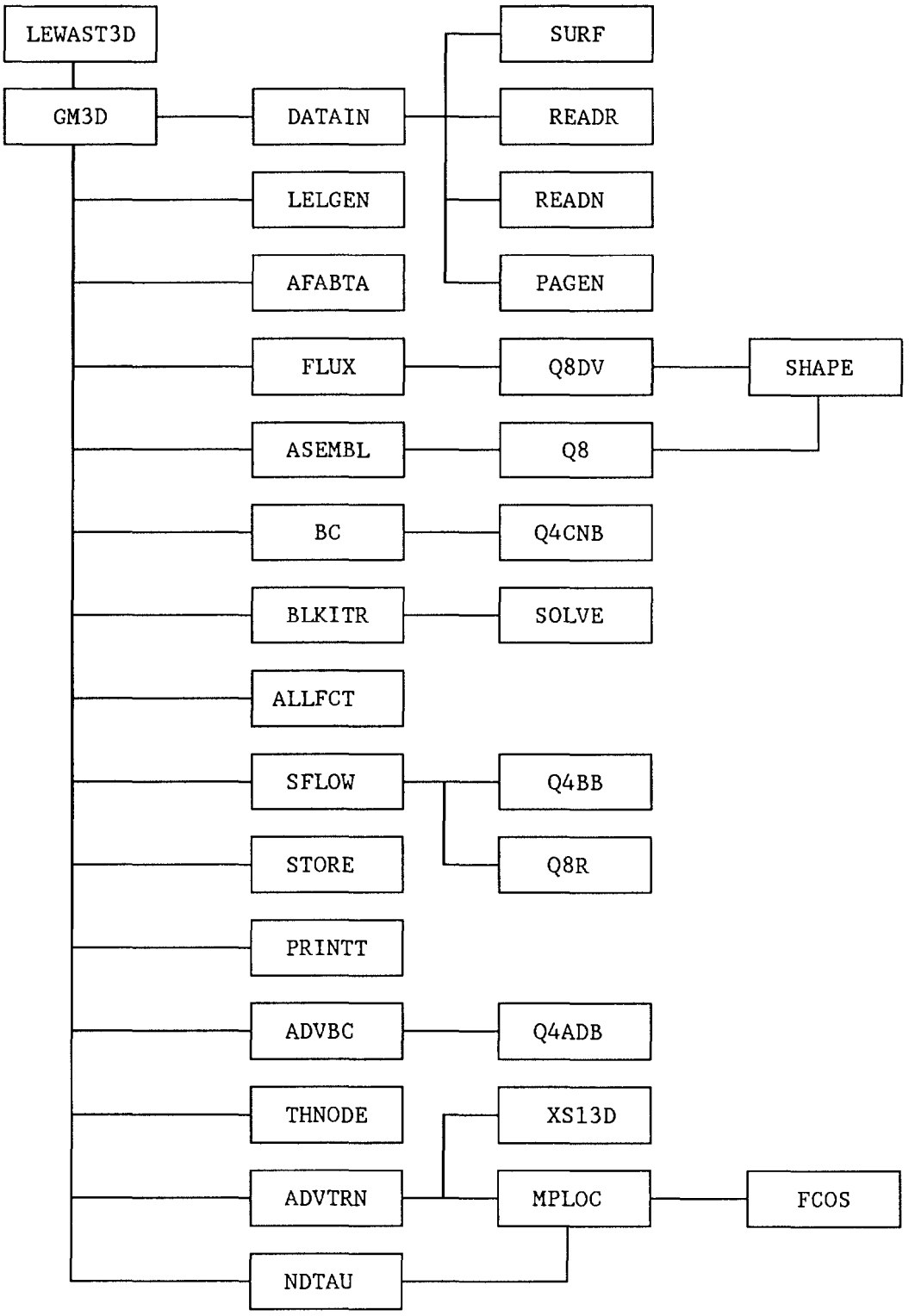

Figure A.2. Program structure of 3DLEWASTE

TABLE A-2. SUBROUTINES INCLUDED IN 3DLEWASTE

Subroutine	Called By	Description
ADVBC	GM3D	Applies specified-flux (Cauchy), variable, and Dirichlet boundary conditions.
ADVTRN	GM3D	Computes the Lagrangian concentrations at all nodes and finds in which element the fictitious particle is located.
AFABTA	GM3D	Calculates the values of the upstream weighting factors along the 12 sides of all elements.
ALLFCT	GM3D	Interpolates functional values for source/sink and boundary conditions.
ASEMBL	GM3D	Evaluates the element matrices and then sums over all element matrices to form a global matrix equation governing the concentration distribution at all nodes.
BC	GM3D	Incorporates Dirichlet, variable composite, specified-flux (Cauchy), and specified-dispersive-flux (Neumann) boundary conditions.
BLKITR	GM3D	Solves the matrix equations with block iteration methods.
DATMN	GM3D	Reads and prints system parameters, geometry, boundary and initial conditions, and properties of the solute and media.
FLUX	GM3D	Evaluates the element matrices and the derivatives of concentrations and then sums over all element matrices to form a matrix equation governing the flux components at all nodal points.
GM3D	LEWAST3D	Controls the entire sequence of operations. Performs either the steady-state computation alone, or a transient- state computation using the steady-state solution as the initial condition, or a transient computation using user-supplied initial conditions.

TABLE A-2. SUBROUTINES INCLUDED IN 3DLEWASTE (continued)

Subroutine	Called By	Description
LELGEN	GM3D	Finds the elements connecting to each node.
MPLOC	NDTAU, ADVTRN	Locates the fictitious particle associated with a particular node. Computes the product of the outward unit vector with the vector from a node on the surface to the fictitious particle.
NDTAU	GM3D	Determines the number of subtime steps and the subtime step size for Lagrangian integration.
PAGEN	DATAIN	Preprocesses pointer arrays that are needed to store the global matrix in compressed form and to construct the subregional block matrices.
PRINTT	GM3D	Prints material flow, concentration, and material flux output as specified by the parameter KPR.
Q4ADB	ADVBC	Implements Dirichlet, specified-flux (Cauchy), and variable boundary conditions in the Lagrangian step computation.
Q4BB	SFLOW	Computes normal flow rates (M/T) by integrating the normal fluxes ($M/L^2/T$) over a boundary surface.
Q4CNB	BC	Computes the boundary-surface matrix and the boundary-surface load vector over a boundary surface.
Q8	ASEMBL	Computes element matrices and element load vectors.
Q8DV	FLUX	Computes the integration of N(I)*N(J) and -N(I)*D>GRAD(C) over an element.
Q8R	SFLOW	Computes the material integration and element source integration over an element.
READN	DATAIN	Automatically generates integer input if required.

TABLE A-2. SUBROUTINES INCLUDED IN 3DLEWASTE (concluded)

Subroutine	Called By	Description
READR	DATAIN	Automatically generates real number input if required.
SFLOW	GM3D	Computes the flux rates through various types of boundaries and the rate at which material increases in the region of interest.
SHAPE	Q8DV, Q8	Computes the base and weighting functions, their derivatives with respect to X, Y, Z, and the Jacobian at a Gaussian point.
SOLVE	BLKITR	Solves a matrix equation with a band matrix solver.
STORE	GM3D	Stores pertinent quantities on a auxiliary device for future uses (e.g., for plotting).
SURF	DATAIN	Identifies the boundary sides and sequences of the boundary nodes, and computes the directional cosine of the surface sides.
THNODE	GM3D	Computes moisture content at a node.
XSI3D	ADVTRN	Computes the local coordinate of an element given the global coordinate within that element.

TABLE A-3. FUNCTIONS INCLUDED IN 3DLEWASTE

Function	Called By	Description
FCOS	MPLOC	Computes the inner product of an outward normal of the surface with a vector connecting a point on the surface and the fictitious particle to determine if the fictitious particle lies inside the surface.

the implementation for such a boundary segment is bypassed. For variable boundaries, if the flow is directed into the region, the concentration of incoming fluid is specified. The Lagrangian concentration is then calculated as:

$$C_i^* = \int_{B_v^-} N_i V_n C_{in} dB / \int_{B_v^-} N_i V_n dB \qquad \text{(A-12)}$$

where

C_i^* = Lagrangian concentration at the boundary node i
V_n = normal vertically integrated Darcy velocity
C_{in} = concentration of incoming fluid
B = global boundary of the region of interest
N_i^e = basis function for nodal point i of element e

Specified-flux (Cauchy) boundary conditions are normally applied to the boundary where flow is directed into the region, where the material flux of incoming fluid is specified. The Lagrangian concentration is thus calculate as:

$$C_i^* = \int_{B_c} N_i q_c dB / \int_{B_c} N_i V_n dB \qquad \text{(A-13)}$$

where C," is the Lagrangian concentration at the boundary node i and q_c is the Cauchy flux of the incoming fluid.

A.2.2 Subroution ADVTRN

This subroutine is called by GM3D to compute the Lagrangian concentrations at all nodes. It calls subroutine MPLOC to find which element a fictitious particle is located in. It also calls subroutine XS13D to compute the local coordinate, given the global coordinate, of the fictitious particle. If the fictitious particle associated with a particular node is located in the interior of the region, the Lagrangian concentration is is obtained by finite element interpolation of the concentration at the previous time step. If the fictitious particle associated with a particular node is outside the region of interest, the Lagrangian concentration is set equal to the previous time-step concentration of the boundary node that is closest to the fictitious particle.

A.2.3 Subroutine AFABTA

This subroutine, which is called by subroutine GM3D, calculates the values of upstream weighting factors along 12 sides of all elements.

A.2.4 Subroutine ALLFCT

This subroutine is called by subroutine GM3D to compute values for all the source/sink and boundary nodes and elements. It uses linear interpolation of tabular data to simulate variations in time for these conditions.

A.2.5 Subroutine ASEMBL

This subroutine is called by subroutine GM3D. After calling subroutine Q8 to evaluate the element matrices, it sums over all element matrices to form a global matrix equation governing the concentration distribution at all nodes.

A.2.6 Subroutine BC

This subroutine, which is called by subroutine GM3D, incorporates Dirichlet, variable composite, specified-flux, and specified-dispersive flux boundary conditions. For a Dirichlet boundary condition, an identity algebraic equation is generated for each Dirichlet nodal point. Any other equation having this nodal variable is modified accordingly to simplify the computation. For a variable composite surface, the integration of the normal velocity times the incoming concentration is added to the load vector and the integration of normal velocity is added to the matrix. For the specified-flux boundaries, the integration of flux is added to the load vector and the integration of normal velocity is added to the matrix. For a specified-dispersive-flux boundary, the integration of gradient flux is added to the load vector.

A.2.7 Subroutine BLKITR

This subroutine is called by subroutine GM3D to solve the matrix equation with block iteration methods. For each subregion, a block matrix equation is constructed based on the global matrix equation and two pointer arrays, GNPLR and LNOJCN (see subroutine PAGEN). The resulting block matrix equation is solved with the direct band matrix solver by calling subroutine SOLVE. This is done for all subregions for each iteration until a convergent solution is obtained.

A.2.8 Subroutine DATAIN

Subroutine DATAIN is called by subroutine GM3D. It reads and prints all data input described in the Section 4.2 except data set 1. It also calls subroutine SURF to identify the boundary segments and boundary nodes and subroutines READR and READN, respectively, to automatically generate real and integer numbers.

A.2.9 Subroutine FLUX

This subroutine is called by subroutine GM3D. It calls subroutine Q8DV to evaluate the element matrices and the derivatives of concentrations. It then sums over all element matrices to form a matrix equation governing the flux components at all nodal points. To save computational time, the matrix is diagonalized by lumping. The flux components due to dispersion can thus be solved point by point. The flux due to velocity is then added to the computed flux due to dispersion. The computed total flux field is then returned to GM3D through the argument.

A.2.1O Subroutine GM3D

The subroutine GM3D controls the entire sequence of operations. It performs either a steady-state computation alone (KSS = 0 and NTI = 0), or a transient- state computa-

tion using the steady-state solution as the initial condition (KSS = 0, NTI > 0), or a transient computation using user-supplied initial conditions (KSS = 1, NTI > 0).

GM3D calls subroutine DATAIN to read and print input data; subroutine LELGEN to generate the pointer array element stencil that describes all elements connected to any node; subroutine ALLFCT to obtain sources/sinks and boundary values; subroutine AFABTA to obtain the upstream weighting factor based on velocity and dispersivity (the upstream weighting factor is needed for solving the steady-state option of 3DLEWASTE); subroutine FLUX to compute material flux; subroutine ASEMBL to assemble the element matrices over all elements; subroutine BC to implement the boundary conditions; subroutine BLKITR to solve the resulting matrix equations with block iteration methods; subroutine SFLOW to calculate flux through all types of boundaries and the water accumulated in the media; subroutine PRINTT to print out the results; subroutine STORE to store the results for plotting; subroutine THNODE to compute the value of moisture content plus bulk density times distribution coefficient in the case of a linear isotherm, or the moisture content in the case of a nonlinear isotherm at all nodes; subroutine NDTAU to compute the number of subtime steps nd the subtime step sizes used for integration in the Lagrangian step; ADVTRN to compute the Lagrangian concentrations at all nodes; and subroutine ADVBC to implement boundary conditions in the Lagrangian step.

A.2.11 Subroutine LELGEN

This subroutine is called by subroutine GM3D to preprocess the pointer array (the global elements stencil), LRL(K,N), where LRL(K,N) is the global element number of the K-th element connected to the global node N. This pointer array is generated based on the element connectivity IE(M,J). Here IE(M,J) is the global node number of the J-th node of element M. This pointer array is needed to facilitate the location of fictitious particles.

A.2. 12 Subroutine MPLOC

This subroutine is called by NDTAU and ADVTRN to locate the fictitious particle associated with a particular node. It uses the function FCOS to compute the product of the outward unit vector with the vector from a node on the surface to the fictitious particle.

A.2.13 Subroutine NDTAU

This subroutine is called by GM3D to compute the subtime-step size and the number of subtime steps such that no fictitious particle travels over an element within a subtime step. The subtime-step size and the number of subtime steps are used in subroutine ADVTRN.

A.2.14 Subroutine PAGEN

This subroutine is called by subroutine DATAIN to preprocess pointer arrays that are needed to store the global matrix in compressed form and to construct the subregional block matrices. The pointer arrays automatically generated in this subroutine include the global node connectivity (stencil), GNOJCN(J,N), regional node connectivity,

LNOJCN(J,I,K), total node number for each subregion, NTNPLR(K), the bandwidth indicator for each subregion, LM.AXDF(K), and a partial fill-up for the mapping array between global node number and local subregion node number, GNPLR(I,K), with I = NNPLR(K) + 1 to NTNPLR(K). Here GNOJCN(J,N) is the global node number of the J-th node connected to the global node N; LNOJN(J,I,K) is the local node number of the J-th node connected to the local node I in K-th subregion; NTNPLR(K) is the total number of nodes in the the K-th subregion, including the interior nodes, the global boundary nodes, and intra-boundary nodes; LMAXDF(K) is the maximum difference between any two nodes of any element in the K-th subregion; and GNPLR(I,K) is the global node number of the I-th local-region node in the K-th subregion. These pointer arrays are generated based on the element connectivity, IE(M,J), the number of nodes for each subregion, NNPLR(K), and the mapping between global node and local-region node, GNLR(I,K), with I = 1, NNPLR(K). Here IE(M,J) is the global node number of the J-th node of element M; NNPLR(K) is the number of nodes in the K-th subregion, including the interior nodes and the global boundary nodes, but not the intraboundary nodes.

A.2. 15 Subroutine PRINTT

This subroutine, which is called by GM3D, is used to line-print the simulation results. These include the fluxes through variable boundary surfaces, the concentration, and vertically integrated material flux components.

A.2.16 Subroutine Q4ADB

This subroutine is called by subroutine ADVBC and implements Dirichlet, specified-flux, and variable boudary conditions in a Lagrangian step computation.

A.2.17 Subroutine Q4BB

This subroutine is called by subroutine SFLOW to perform surface integration of the following type:

$$RRQ(I) = \int_{B_e} N_i \cdot F \, dB \qquad \text{(A-14)}$$

where F is the normal flux and RRQ(I) is a 3DLEWASTE program variable.

A.2.18 Subroutine Q4CNB

This subroutine is called by the subroutine BC to compute the surface node flux of the type:

$$RQ(I) = \int_{B_e} N_i^e q \, dB \tag{A-15a}$$

where q is either the specified- (or Cauchy) flux, specified-dispersive- (or Neumann) flux, or $\mathbf{n} \cdot \mathbf{V} C_v$; and RQ(I) is a 3DLEWASTE program variable. It also computes the boundary element matrices:

$$BQ(I,J) = \int_{B_e} N_i^e \mathbf{V} N_j^e \, dR \tag{A-15b}$$

where N_j^e is the basis function for nodal point j of element e, R is the region of interest, V is the Darcy velocity, and BQ(I,J) is a 3DLEWASTE program variable.

A.2. 19 Subroutine Q8

This subroutine is called by the subroutine ASEMBL to compute the element matrix given by

$$QA(I,J) = \int_{R_e} N_i^e \theta N_j^e \, dR \tag{A-16a}$$

$$QAA(I,J) = \int_{R_e} N_j^e \rho_b \frac{dS}{dC} N_i^e \, dR \tag{A-16b}$$

$$QB(I,J) = \int_{R_e} (\nabla N_i^e) \cdot \theta \mathbf{D} \cdot (\nabla N_j^e) \, dR \tag{A-16C}$$

$$QV(I,J) = \int_{R_e} N_i^e \mathbf{V} \cdot (\nabla N_j^e) \, dR \tag{A-16d}$$

$$QC(I,J) = \int_{R_e} N_i^e [\lambda(\theta + \rho_b \frac{dS}{dC}) + Q] N_j^e \, dR \tag{A-16e}$$

where

C_w = dissolved concentration at the previous iteration
$\mathbf{D}$ = dispersion coefficient tensor
θ = moisture content
S = species concentration in the adsorbed phase
Q = source rate of water
ρ_b = bulk density of the porous medium
λ = material decay constant
∇ = del operator indicating gradient
$\nabla\cdot$ = del operator indicating divergence

and where QA(I,J), QAA(I,J), QB(I,J), QV(I,J), and QC(I,J) are 3DLEWASTE program variables. Note that dS/dC should be evaluated at C_w. Subroutines Q8 also calculates the element load vector given by:

$$QR(I) = \int_{R_e} N_i^e [-\lambda \rho_b (S_w - \frac{dS}{dC} C_w) + QC_{in}] dR \qquad \text{(A-16f)}$$

where C_w and SW are the dissolved and adsorbed concentrations at the previous iteration, respectively, and QR(I) is a program variable.

A.2.20 Subroutine Q8DV

Subroutine Q8DV is called by subroutine FLUX to compute the element matrices given by:

$$QB(I,J) = \int_{R_e} N_i^e N_j^e dR \qquad \text{(A-17a)}$$

Subroutine Q8DV also evaluates the element load vector:

$$QRX(I) = -\int_{R_e} N_i^e \mathbf{i} \cdot \theta \mathbf{D} \cdot (\nabla N_j^e) C_j dR \qquad \text{(A-17b)}$$

$$QRY(I) = -\int_{R_e} N_i^e \mathbf{j} \cdot \theta \mathbf{D} \cdot (\nabla N_j^e) C_j dR \qquad \text{(A-17c)}$$

$$QRZ(I) = -\int_{R_e} N_i^e \mathbf{k} \cdot \theta \mathbf{D} \cdot (\nabla N_j^e) C_j dR \qquad \text{(A-17d)}$$

where

C_j = concentration at nodal point j
$\mathbf{i}$ = unit vector along the x-direction
$\mathbf{j}$ = unit vector along the y-coordinate
$\mathbf{k}$ = unit vector along the z-coordinate

and where QRX(I), QRY(I), AND QRZ(I) are program variables.

A.2.21 Subroutine Q8R

This subroutine, which is called by subroutine SFLOW, is used to compute contributions to FRATE(8), FRATE(9), FRATE(l), and FRATE(14), discussed in Section A.2.24, by performing material integration and element source integration over an element.

$$QRM = \int_R \theta C dR \tag{A-18a}$$

$$QDM = \int_R S dR \tag{A-18b}$$

$$SOSM = \int_R [QC_{in}(1+sign(Q)) + QC(1-sign(Q))]/2 dR \tag{A-18c}$$

where QRM, QDM, and SOSM are 3DLEWASTE program variables.

A.2.22 Subroutine READN

This subroutine is called by subroutine DATAIN to generate integer numbers for the input data sets if required.

A.2.23 Subroutine READR

This subroutine is called by subroutine DATAIN to automatically generate real numbers for the input data sets if required. Automatic generation-of regularly patterned data is built into this subroutine.

A.2.24 Subroutine SFLOW

This subroutine is called by subroutine GM3D. It is used to compute flux rates through various types of boundaries and the rate at which material increases in the region of interest. In this subroutine, the variable FRATE(7) stores the flux through the whole boundary. It is given by

$$FRATE(7) = \int_{B} (F_x n_x + F_y n_y) dB \qquad \text{(A-19)}$$

where B is the global boundary of the region of interest; F_x, and F_y are the vertically integrated flux components and n_x and n_y are the directional cosines of the outward unit vector normal to the boundary B. FRATE(1) stores the flux rates through a Dirichlet boundary B_d. FRATE(2) and FRATE(3) store the flux rate through specified-flux (Cauchy) and specified-dispersive-flux (Neumann) boundaries, respectively.

$$FRATE(1) = \int_{B_d} (F_x n_x + F_y n_y) dB \qquad \text{(A-20a)}$$

$$FRATE(2) = \int_{B_c} (F_x n_x + F_y n_y) dB \qquad \text{(A-20b)}$$

$$FRATE(3) = \int_{B_n} (F_x n_x + F_y n_y) dB \qquad \text{(A-20c)}$$

FRATE(4) and FRATE(5) store incoming flux and outgoing flux rates, respectively, through the variable boundaries B, and B_v^+, as given by:

$$FRATE(4) = \int_{B_{v^-}} (F_x n_x + F_y n_y) dB \qquad \text{(A-20d)}$$

$$FRATE(5) = \int_{B_{v^+}} (F_x n_x + F_y n_y) dB \qquad \text{(A-20e)}$$

where B_{V^-} and B_{V^-} are that part of variable boundary where the fluxes are directed into the region and out from the region, respectively. The integration of Equations A-20a through A-20e is carried out by the subroutine Q4BB.

FRATE(6), which is related to the numerical loss, is given by:

$$FRATE(6)=FRATE(7)-\sum_{I=1}^{5} FRATE(I) \tag{A-21}$$

FRATE(8) and FRATE(9) store the accumulate rate in the dissolved and adsorbed phases, respectively, as given by:

$$FRATE(8)=\int_R \theta C dR \tag{A-22}$$

$$FRATE(9)=\int_R \rho_b S dR \tag{A-23}$$

FRATE(10) stores the rate loss due to decay and FRATE(11) through FRATE(13) are set to zero as given by:

$$FRATE(10)=\int_R \lambda(\theta C+\rho_b S)dR \tag{A-24}$$

$$FRATE(11)=FRATE(12)=FRATE(13)=0 \tag{A-25}$$

FRATE(14) is used to store the source/sink rate as:

$$FRATE(14)=\int_R [QC_{in}(1+sign(Q))+QC(1-sign(Q))]/2dR \tag{A-26}$$

If there is no numerical error in the computation, the following equation should be satisfied:

$$\sum_{I=7}^{14} FRATE(I)=0 \tag{A-27}$$

and FRATE(6) should be equal to zero.

A.2.25 Subroutine SHAPE

This subroutine is called by subroutines Q8DV and Q8 to evaluate the value of the base and weighting functions and their derivatives at a Gaussian point.

A.2.26 Subroutine SOLVE

This subroutine is called by the subroutine BLKITR to solve a matrix equation of the type:

$$[C]\{x\}=\{y\} \tag{A-28}$$

where [C] is the coefficient matrix and {x) and {y) are two vectors. {x) is the unknown to be solved, and {y) is the known load vector. The computer returns the solution {y) and stores it in {y). The computation is a standard banded Gaussian direct elimination procedure.

A.2.27 Subroutine STORE

This subroutine, which is called by subroutine GM3D, stores the simulation results in a binery file for use in plotting. The information stored includes regional geometry, concentrations, and vertically integrated material flux components at all nodes for any desired time step.

A.2.28 Subroutine SURF

Subroutine SURF is called by subroutine DATAIN. It identifies the boundary sides, sequences the boundary nodes, and computes the directional cosine of the surface sides. The mappings from boundary nodes to global nodes are stored in NPBB(I) (where NPBB(I) is the global node number of the I-th boundary node). The boundary node numbers of the four nodes for each boundary side are stored in ISB(I,J) (where ISB(I,J) is the boundary node number of the I-th node of the J-th side, I = 1 to 4). There are six sides for each element. Which of these six sides is the boundary side is determined automatically in the subroutine SURF and is stored in ISB(5,J). The global element number, to which the J-th boundary side belongs, is also preprocessed in the subroutine SURF and is stored in ISB(6,J). The directional cosines of the J-th boundary side are computed and stored in DCOSB(I,J) (where DCOSB(I,J) is the directional cosine of the J-th surface with I-th coordinate, I = 1 to 3). The information contained in NPBB, ISB, and DOSB, along with the number of boundary nodes and the number of boundary sides is returned to subroutine DATAIN for other uses.

A.2.29 Subroutine THNODE

This subroutine is called by GM3D to compute $(\theta+\rho_b dS/dC)$ for the linear isotherm model or θ for the Freundlich and Langmuir nonlinear isotherm models.

A.2.30 Subroutine XSI3D

This subroutine is called by ADVTRN to compute the local coordinate of an element given the global coordinate within that element. With the local coordinate, the Lagrangian concentration can then easily be interpolated from those on the nodes of the element.

APPENDIX B

INPUT AND OUTPUT DEVICES

TABLE B-1. LOGICAL UNITS USED IN 3DFEMWATER

Logical Unit	Number	Purpose
LUSTO	11	Logical unit for storing binary output for use in 3DLEWASTE or for plotting purposes.
LUBAR	13	Logical unit for storing binary boundary arrays, if they are generated in the present job, for use in subsequent executions of the same scenario.
LUPAR	14	Logical unit for storing binary pointer arrays, if they are generated in the present job, for use in subsequent executions of the same scenario.
LUINP	15	Logical unit for reading input data.
LUOUT	16	Logical unit for writing output data.

TABLE B-2. LOGICAL UNITS USED IN 3DLEWASTE

Logical Unit	Number	Purpose
LUFLW	11	Logical unit for reading flow data from the 3DFEMWATER simulation.
LUSTO	12	Logical unit for storing binary output for use in 3DLEWASTE or for plotting purposes.
LUBAR	13	Logical unit for storing binary boundary arrays, if they are generated in the present job, for use in subsequent executions of the same scenario.
LUPAR	14	Logical unit for storing binary pointer arrays, if they are generated in the present job, for use in subsequent executions of the same scenario.
LUINP	15	Logical unit for reading input data.
LUOUT	16	Logical unit for writing output data.

APPENDIX C

DEFAULT VALUES FOR THE MAXIMUM CONTROL PARAMETERS

TABLE C-1. MAXIMUM CONTROL PARAMETERS USED IN 3DFEMWATER

Parameter	Definition	Default Value	Location
Maximum Control-Integers for the Spatial Domain			
MAXNPK	Maximum Number of Nodes	25578	PMXSD.INC
MAXELK	Maximum Number of Elements	22080	PMXSD.INC
MXBESK	Maximum Number of Boundary-Element Surfaces	7138	PMXSD.INC
MXBNPK	Maximum Number of Boundary Nodal Points	7140	PMXSD.INC
MXJBDK	Maximum Number of Nonzero Elements in Any Row	27	PMXSD.INC
MXKBDK	Maximum Number of Elements Connecting to Any Node	8	PMXSD.INC
Maximum Control-Integers for the Time Domain			
MXNTIK	Maximum Number of Time Steps	100	PMXTD.INC
MXDTCK	Maximum Number of DELT Changes	10	PMXTD.INC
Maximum Control-Integers for Subregions			
LTMXNK	Maximum Number of Total Nodal Points in any Subregion, Including Interior Nodes, Global Boundary Nodes, and Intraboundary Nodes	3654	PMXSR.INC
LMXNPK	Maximum Number of Nodal Points in any Subregion Including Interior Nodes and Global Boundary Nodes	1218	PMXSR.INC
LMXBWK	Maximum Number of the Bandwidth in any Subregion	59	PMXSR.INC
MXRGNK	Maximum Number of Subregions	21	PMXSRJNC
Maximum Control-Integers for Source/Sinks			
MXSELK	Maximum Number of Source Elements	1	PMXSS.INC
MXSPRK	Maximum Number of Source Profiles	1	PMXSS.INC
MXSDPK	Maximum Number of Data Points on Each Element Source/Sink Profile	1	PMXSS.INC
MXWNPK	Maximum Number of Point (Well) Nodal Points	2	PMXSS.INC
MXWPRK	Maximum Number of Point (Well) Source/Sink Profiles	2	PMXSS.INC
MXWDPK	Maximum Number of Data Points on Each Point (Well) Source/Sink Profile	2	PMXSS.INC

(continued)

TABLE C-1. MAXIMUM CONTROL PARAMETERS USED IN 3DFEMWATER (concluded)

Parameter	Definition	Default Value	Location
Maximum Control-Integers for Specified-Flux (Cauchy) Boundary Conditions			
MXCNPK	Maximum Number of Specified-Flux Nodal Points	147	PMXCB.INC
MXCESK	Maximum Number of Specified-Flux Element Surfaces	120	PMXCB.INC
MXCPRK	Maximum Number of Specified-Flux Profiles	1	PMXCB.INC
MXCDPK	Maximum Number of Data Points on Each Specified-Flux Profile	2	PMXCB.INC
Maximum Control-Integers for Specified-Pressure-Head Gradient Boundary Conditions			
MXNNPK	Maximum Number of Specified-Pressure-Head Gradient Nodal Points	1	PMXNB.INC
MXNESK	Maximum Number of Specified-Pressure-Head Gradient Element Surfaces	1	PMXNB.INC
MXNPRK	Maximum Number of Specified-Pressure-Head Gradient Flux Profiles	1	PMXNB.INC
MXNDPK	Maximum Number of Data Points on Each Specified-Pressure-Head Gradient Flux Refile	2	PMXNB.INC
Maximum Control-Integers for Variable (Rainfall/Evaporation-Seepage) Boundary Conditions			
MXVNPK	Maximum Number of Variable Nodal Points	2079	PMXRSB.INC
MXVESK	Maximum Number of Variable Element Surfaces	1960	PMXRSB.INC
MXVPRK	Maximum Number of Rainfall Refiles	2	PMXRSB.INC
MXVDPK	Maximum Number of Data Point on Each Rainfall Profile	2	PMXRSB.INC
Maximum Control-Integers for Dirichlet Boundary Conditions			
MXDNPK	Maximum Number of Dirichlet Nodal Points	210	PMXDB.INC
MXDPRK	Maximum Number of Dirichlet Total Head Profiles	2	PMXDB,INC
MXDDPK	Maximum Number of Data Points on Each Dirichlet Profile	2	PMXDB.INC
Maximum Control-Integers for Material and Soil Properties			
MXMATK	Maximum Number of Material Types	6	PMXMS.INC
MXSPMK	Maximum Number of Soil Parameters Per Material to Describe Soil Characteristic Curves	5	PMXMS.INC
MXMPMK	Maximum Number of Material Properties per Material	6	PMXMS.INC

TABLE C-2. MAXIMUM CONTROL PARAMETERS USED IN 3DLEWWASTE

Parameter	Definition	Default Value	Location
Maximum Control-Integers for the Spatial Domain			
MAXNPK	Maximum Number of Nodes	25578	PMXSD.INC
MAXELK	Maximum Number of Elements	22080	PMXSD.INC
MXBESK	Maximum Number of Boundary-Element Surfaces	7138	PMXSD.INC
MXBNPK	Maximum Number of Boundary Nodal Points	7140	PMXSD.INC
MXJBDK	Maximum Number of Nonzero Elements in Any Row	27	PMXSD.INC
MXKBDK	Maximum Number of Elements Connecting to Any Node	8	PMXSD.INC
Maximum Control-Integers for the Time Domain			
MXNTIK	Maximum Number of Time Steps	500	PMXTD.INC
MXDTCK	Maximum Number of DELT Changes	20	PMXTD.INC
Maximum Control-Integers for Subregions			
LTMXNK	Maximum Number of Total Nodal Points in any Subregion, Including Interior Nodes, Global Boundary Nodes, and Intraboundary Nodes	3654	PMXSR.INC
LMXNPK	Maximum Number of Nodal Points in any Subregion, Including Interior Nodes and Global Boundary Nodes	1218	PMXSR.INC
LMXBWK	Maximum Number of the Bandwidth in any Subregion	59	PMXSR.INC
MXRGNK	Maximum Number of Subregions	21	PMXSR.INC
Maximum Control-Integers for Source/Sinks			
MXSELK	Maximum Number of Source Elements	180	PMXSS.INC
MXSPRK	Maximum Number of Source Profiles	1	PMXSS.INC
MXSDPK	Maximum Number of Data Points on Each Element Source/Sink Profile	8	PMXSS.INC
MXWNPK	Maximum Number of Point (Well) Nodal Points	1	PMXSS.INC
MXWPRK	Maximum Number of Point (Well) Source/Sink Profiles	1	PMXSS.INC
MXWDPK	Maximum Number of Data Points on Each Point (Well) Source/Sink Profile	4	PMXSS.INC

(continued)

TABLE C-2. MAXIMUM CONTROL PARAMETERS USED IN3DLEWWASTE (concluded)

Parameter	Definition	Default Value	Location
Maximum Control-Integers for Specified-Flux (Cauchy) Boundary Conditions			
MXCNPK	Maximum Number of Specified-Flux Nodal Points	8	PMXCB.INC
MXCESK	Maximum Number of Specified-Flux Element Surfaces	2	PMXCB.INC
MXCPRK	Maximum Number of Specified-Flux Profiles	2	PMXCB.INC
MXCDPK	Maximum Number of Data Points on Each Specified-Flux Profile	4	PMXCB.INC
Maximum Control-Integers for Specified-Dispersive-Flux Boundary Conditions			
MXNNPK	Maximum Number of Specified-Dispersive-Flux Nodal Points	8	PMXNB.INC
MXNESK	Maximum Number of Specified-Dispersive-Flux Element Surfaces	2	PMXNB.lNC
MXNPRK	Maximum Number of Specified-Dispersive-Flux Profiles	2	PMXNB.INC
MXNDPK	Maximum Number of Data Points on Each Specified-Dispersive-Flux Profile	4	PMXNB.INC
Maximum Control-Integers for Variable (Run-In/Flow-Out) Boundary Conditions			
MXVNPK	Maximum Number of Variable Nodal Points	38	PMXRSB.INC
MXVESK	Maximum Number of Variable Element Surfaces	18	PMXRSB.INC
MXVPRK	Maximum Number of Rainfall Profiles	2	PMXRSB.INC
MXVDPK	Maximum Number of Data Point on Each Rainfall Profile	4	PMXRSB.INC
Maximum Control-Integers for Dirichlet Boundary Conditions			
MXDNPK	Maximum Number of Dirichlet Nodal Points	81	PMXDB.INC
MXDPRK	Maximum Number of Dirichlet Total Head Profiles	81	PMXDB.INC
MXDDPK	Maximum Number of Data Points on Each Dirichlet Profile	2	PMXDB.INC
Maximum Control-Integers for Material			
MXMATK	Maximum Number of Material Types	6	PMXMS,INC
MXMPMK	Maximum Number of Material Properties per Material	8	PMXMS.INC

APPENDIX D

PROGRAM VARIABLE DESCRIPTIONS

Information about the program variables is given in two tables in this appendix. 3DFEMWATER program variables are listed in Table D-1 and 3DLEWASTE program variables are shown in Table D-2. In the tables, the definition, type, and units of each variable are provided. In addition, the tables indicate 1) the subroutines associated with each variable and 2) whether a variable is an input (I), output (0), or modified (M) variable in the subroutines. Also, if a variable is included in a COMMON block, the COMMON block name is given.

COMMON blocks are used in 3DFEMWATER/3DLEWASTE to minimize the use of subroutine arguments. Each COMMON block, which contains related variables, is stored as a file separate from the 3DFEMWATER/3DLEWASTE code and is accessed by the use of INCLUDE statements at the beginning of the main program and each subroutine. Only those COMMON blocks needed for the execution of a subroutine are included in the subroutine.

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
AGRAV	--	Scalar	Gravity Term Included? 0.0 = no, 1.0 = yes	Q8		I
AKPROP (I,J)	L/T	Array	I-th Parameter to Describe the Relative Conductivity as a Function of Pressure Head for the J-th Material or the I-th Data Point of Relative Conductivity for the J-th Material	GW3D DATAIN SPROP		M O I
AKR(I,M)	--	Array	Relative Conductivity at the I-th Node of the M-th Element	GW3D VELT SPROP ASEMBL BC		M I O I I
AKXG(8)	L/T	Array	XX-Hydraulic Conductivity at Eight Gaussian Points	Q8DV Q8		I I
AKXYG(8)	L/T	Array	XY-Hydraulic Conductivity at Eight Gaussian Points	Q8DV Q8		I I
AKXZG(8)	L/T	Array	XZ-Hydraulic Conductivity at Eight Gaussian Points	Q8DV Q8		I I
AKYG(8)	L/T	Array	W-Hydraulic Conductivity at Eight Gaussian Points	Q8DV Q8		I I
AKYZG(8)	L/T	Array	YZ-Hydraulic Conductivity at Eight Gaussian Points	Q8DV Q8		I I
AKZG(8)	L/T	Array	ZZ-Hydraulic Conductivity at Eight Gaussian Points	Q8DV Q8		I I
BFLX(I)	L^3/T	Array	Present Time Flux at the I-th Boundary Node	GW3D SFLOW PRINTT'		M M I
BFLXP(I)	L^3/T	Array	Previous Time Flux at the I-th Boundary Node	GW3D SFLOW		M M
C(MAXNP)	L	Array	Final Solution	BLKITR SOLVE		O M
CAPROP (I,J)	1/L	Array	I-th Data Point of Water Capacity for the J-th Material	GW3D DATAIN SPROP		M O I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
CHNG	--	Scalar	Multiplier for Increasing DELT		CREAL	
CMATRX (N,I)	--	Array	An Array to Store the assembled Global Matrix	GW3D VELT ASEMBL BC		M O O M
CMTRXG (MAXNP, JBAND)	--	Array	Global Matrix	BLKITR		I
CMTRXL (N,I)	--	Array	Assembled Matrix for a subregion	GW3D BLKITR		M M
CW(MAXNP)	L	Array		BLKITR		M
DCOSB(l,I)	--	Array	X-Directional Cosine of the I-th Boundary Side	GW3D DATAIN SURF BCPREP BC SFLOW STORE		M O O I I I I
DCOSB(2,1)	--	Array	Y-Directional Cosine of the I-th Boundary Side	GW3D DATAIN SURF BCPREP BC SFLOW STORE		M O O I I I I
DCOSB(3,1)	--	Array	Z-Directional Cosine of the I-th Boundary Side	GW3D DATAIN SURF BCPREP BC SFLOW STORE		M O O I I I I
DCYFLX(NP)	L^3/T	Array	Darcy Flux Through the NP-th Variable Boundary Node	GW3D BCPREP PRINTT		M O I
DELMAX	T	Scalar	Maximum Value of DELT		CREAL	
DELT	T	Scaler	Time Increment	ASEMBL SFLOW PRINTT	CREAL	I I I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARLABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
DELTO	T	Scalar	Time Increment		CREAL	
DHQ(8)	L	Array	Pressure Difference Between the Present Time Step and the Previous Time Step at Eight Nodes of the Element	Q8TH		I
DJAC	L^3	Scalar	Determinant of the Jacobian	BASE		O
DNX(8)	IL	Array	Partial Derivative of the Base Function with Respect to x	BASE		O
DNY(8)	1/L	Array	Partial Derivative of the Base Function with Respect to y	BASE		O
DNZ(8)	l/L	Array	Partial Derivative of the Base Function with Respect to z	BASE		O
DTH(I,M)	l/L	Array	Water Capacity at the I-th Node of the M-th Element	GW3D SPROP ASEMBL SFLOW		M O I I
DTHG(8)	1/L	Array	Water Capacity at Eight Gaussian Points of the Element	Q8		I
F(MAXNOD)	--	Array	Array of Real Numbers that are to be Read and Generated Automatically	READR		O
FLOW(10)	L^3	Array	Increment of Flow		CFLOW	
FLX(NP)	L3iT	Array	Rainfall Flux Through the NP-th VB Node	GW3D BCPREP BC		M O I
FRATE(10)	L^3/T	Array	Flow Rate		CFLOW	
F1Q(4)	L3/ql/L2	Array	Specified Normal Flux at Four Nodes of the Surface	Q4S		I
F2Q(4)	$L^3/T/L^2$	Array	Gravity Flux at Four Nodes of a Specified-Pressure-Head Gradient (Neumann) Surface	Q4S		I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
GNLR(I,K)	--	Array	Global Node Number of the I-th Node in the K-th Subregion	GW3D DATAIN PAGEN BLKITR STORE		M 0 M I I
H(N)	L	Array	Pressure Head at the Present Time	GW3D DATAIN VELT		0 0 I
HCON(NP)	L	Array	Pending Depth of the NP-th Variable Boundary Node	GW3D DATAIN BCPREP BC		M 0 I I
HDB(J)	L	Array	Total Head of the J-th Profile at the Present Time	GW3D BC		M I
HDBF(I,J)	L	Arr	Total Head of the I-th Data Point in the J-th Profile	GW3D DATAIN		M 0
HMIN(NP)	L	Array	Minimum Pressure Allowed for the NP-th VB Node	GW3D DATAIN BCPREP BC		M 0 I I
HP(N)	L	Arr	Previous-Time Pressure Head at the N-th Node	GW3D ASEMBL		M I
HPROP(I,J)	L	Array	I-th Data Point of Pressure for the J-th Material	GW3D DATAIN SPROP		M 0 I
HT(N)	L	Array	Total Head the N-th Node	GW3D PRIN'lT STORE VELT		M I I 0
HTQ(8)	L	Arr	Total Head at Eight Nodes of the Element	Q8DV		I
HW(N)	L	Array	Nonlinear Pressure Head Iterate at the N-th Node	GW3D		M
IBUG	--	Scalar	Diagnostic Print-Out Indicator	BLKITR		I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ICTYP(MP)	--	Array	Type of Specified-Flux (Cauchy) Profile Assigned to the MP-th Side	GW3D DATAIN BC		M O I
IDTYP(NP)	--	Array	Total Head Profile Type of NP-th Dirichlet Node	GW3D DATAIN BC		M O I
IE(M,I)	--	Array	Global Node Number of the I-th Node of the M-th Element if I is Between 1 and 8, Material Type of the M-th Element if I = 9	GW3D DATAIN SURF PAGEN VELT SPROP BCPREP ASEMBL BC SFLOW STORE		M O I I I I I I I I I
IGEOM	--	Scalar	Geometry Description Output Control		CINTE	
IHALFB	--	Scalar	Half Band with Plus 1	SOLVE		I
ILUMP	--	Scalar	Lumping Indicator	Q8	OPTN	I
IMID	--	Scalar	Mid-Difference Indicator		OPTN	
INDTYP(MXTYP)	--	Array	Array of Integers that are to be Read or Generated Automatically	READN		O
INTYP(MP)	--	Array	Type of Specified-Pressure-Head Gradient (Neumann) Flux Profile Assigned to the MP-th Neumam Side	GW3D DATAIN BC		M O I
IRTYP(MP)	--	Array	Type of Rainfall Profile Assigned to the MP-th Variable Boundary Side	GW3D DATAIN BCPREP		M O I
ISB(l,I)	--	Array	Boundary Node Number of the First Node of the I-th Boundary Side	GW3D DATAIN SURF BCPREP BC SFLOW STORE		M O O I I I I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Unite	Type	Description	Sub-routine	Common Block	I,M,O
ISB(2,I)	--	Array	Boundary Node Number of the Second Node of the I-th Boundary Side	GW3D		M
				DATAIN		O
				SURF		O
				BCPREP		I
				BC		I
				SFLOW		I
				STORE		I
ISB(3,I)	--	Array	Boundary Node Number of the Third Node of the I-th Boundary Side	GW3D		M
				DATAIN		O
				SURF		O
				BCPREP		I
				BC		I
				SFLOW		I
				STORE		I
ISB(4,I)	--	Array	Boundary Node Number of the Fourth Node of the I-th Boundary Side	GW3D		M
				DATAIN		O
				SURF		O
				BCPREP		I
				BC		I
				SFLOW		I
				STORE		I
ISB(5,I)	--	Array	Element Side Index of the I-th Boundary Side: l=left side, 2=front side, 3=right side, 4=back side, 5=bottom side, 6=top side	GW3D		M
				DATAIN		O
				SURF		O
				BCPREP		I
				BC		I
				SFLOW		I
				STORE		I
ISB(6,I)	--	Array	Element Number to which the I-th Boundary Side Belongs	GW3D		M
				DATAIN		O
				SURF		O
				BCPREP		I
				BC		I
				SFLOW		I
				STORE		I
ISC(l,MP)	--	Array	Global Node Number of the First Node of the MP-th Cauchy Side	GW3D		M
				DATAIN		O
				BC		I
ISC(2,MP)	--	Array	Global Node Number of the Second Node of the MP-th Cauchy Side	GW3D		M
				DATAIN		O
				BC		I
ISC(3,MP)	--	Array	Global Node Number of the Third Node of the MP-th Cauchy Side	GW3D		M
				DATAIN		O
				BC		I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ISC(4,MP)	--	Array	Global Node Number at the Fourth Node of the MP-th Cauchy Side	GW3D DATAIN BC		M O I
ISC(5,MP)	--	Array	Boundary Side Number of the MP-th Cauchy Side	GW3D DATAIN BC		M O I
ISN(l,MP)	--	Array	Global Node Number of the First Node of the MP-th Neumann Side	GW3D DATAIN BC		M O I
ISN(2,MP)	--	Array	Global Node Number of the Second Node of the MP-th Neumann Side	GW3D DATAIN BC		M O I
ISN(3,MP)	--	Array	Global Node Number of the Third Node of the MP-th Neumann Side	GW3D DATAIN BC		M O I
ISN(4,MP)	--	Array	Global Node Number of the Fourth Node of the MP-th Neurnam Side	GW3D DATAIN BC		M O I
ISN(5,MPF)	--	Array	Boundary Side Number of the MP-th Neumann Side	GW3D DATAIN BC		M O I
ISTYP(MP)	--	Array	Source/Sink Type Assigned to the MP-th S/S Element	GW3D DATAIN ASEMBL SFLOW		M O I I
ISV(l,MP)	--	Array	Global Node Number of the First Node of the MP-th Variable Side	GW3D DATAIN BCPREP		M O I
ISV(2,MP)	--	Array	Global Node Number of the Second Node of the MP-th Variable Side	GW3D DATAIN BCPREP		M O I
ISV(3,MP)	--	Array	Global Node Number of the Third Node of the MP-th Variable Side	GW3D DATA.IN BCPREP		M O I
ISV(4,MP)	--	Array	Global Node Number of the Fourth Node of the MP-th Variable Side	GW3D DATAIN BCPREP		M O I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ISV(5,MP)	--	Array	Boundary Node Number of the MP-th VB Side	GW3D DATAIN BCPREP		M O I
ITIM	--	Scalar	Time Step Number	PRINTT		I
IWTYP(NP)	--	Array	Source/Sink Type Assigned to the NP-th Well Node	GW3D DATAIN ASEMBL SFLOW		M O I I
KANALY	--	Scalar	Analytical Input Control	ALLFCT		I
KCAI	--	Scalar	Analytical Specified-Flux (Cauchy) Input Control		CCBC	
KDAI	--	Scalar	Analytical Dirichlet Input Control		CDBC	
KDLAG	--	Scalar	Diagnostic Print-Out Table Number	PRINTT		M
KDSK(I)	--	Array	Auxiliary Output Control for the I-th Time Step; O = no auxiliary output 1 = output stored	GW3D DATAIN		M O
KDSKO	--	Scalar	Disk Output Control		CINTE	
KFLOW	--	Scalar	System Flow Counter	SFLOW		I
KGRAV	--	Scalar	Index of Gravity Control		CGEOM	
KKK	--	Scalar	Decomposition or Back Substitution Indicator 1 = decomposition, 2 = back substitution	SOLVE		
KNAI	--	Scalar	Analytical Neumann Flux Input Control		CNBC	
KOUT	--	Scalar	Prin-Out Table Number	PRINTT		M
KPR(I)	--	Array	Line-printer Control for I-th Time Step: 0 = print nothing 1 = print system mass balance plus above 2 = print pressure head plus above	GW3D DATAIN BLKITR PRIN'M'		M O I I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
			3 = print total head plus above 4 = print moisture content plus above 5 = print Darcy velocity plus above			
KPRO	--	Scalar	Output Control		CINTE	
KRAI	--	Scalar	Analytical Rainfall Input Control		CVBC	
KSAI	--	Scalar	Analytical Distributed Source/Sink Input Control		CS	
KSP	--	Scalar	Soil Property Tabular Input Control	SPROP	CINTE	I
KSS	--	Scalar	Steady-State I.C. Control	ASEMBL	CINTE	I
KWAI	--	Scalar	Analytical Well Source/ Sink Input Control		CW	
LES(MP)	--	Array	Global Element Number of the MP-th S/S Element	GW3D DATAIN ASEMBL SFLOW		M O I I
LMAXDF(K)	--	Array	Maximum Difference Between Eight Nodes of Any Element	GW3D PAGEN BLKITR DATAIN		M O I O
LMXBW	--	Scalar	Maximum No. of the Bandwidth in any Subregion	BLKITR	LGEOM	I
LMXBWK	--	Scalar	Maximum No. of the Bandwidth in Any Subregion			
LMXNP	--	Scalar	Maximum No. of Nodal Points in any Subregion, Including Interior Nodes and Global Boundary Nodes	BLKITR	LGEOM	I
LMXNPK	--	Scalar	Maximum No. of Nodal Points in any Subregion, Including Interior Nodes and Global Boundary Nodes			

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
LNOJCN (J,I,K)	--	Array	Local Node No. of the J-th Compressed Number Connecting to the I-th Local Node in the K-th Subregion	GW3D PAGEN BLKITR DATAIN		M O 1 O
LRL(I,N)	--	Array	Global Element Number of the I-th Element Connecting to the N-th Global Node	GW3D DATAIN SURF PAGEN		M O 1 O
LRN(I,N)	--	Array	Global Node Number of the I-th Node Connecting to the N-th Global Node	GW3D PAGEN ASEMBL BC DATAIN		M O 1 1 O
LTMXNK	--	Scalar	Maximum No. of Total Nodal Points in any Subregion, Including Interior Nodes, and Global Boundary Nodes			
LTMXNP	--	Scalar	Maximum No. of Total Nodal Points in any Subregion, Including Interior Nodes, and Global Boundary Nodes	BLKITR STORE	LGEOM	I I
LUBAR	--	Scalar	Logical Unit for Storing Binary Boundary Arrays	GW3D DATAIN		I I
LUINP	--	Scalar	Logical Unit for Input Data	GW3D DATAIN READR READN		I I I I
LUOUT	--	Scalar	Logical Unit for Output Data	GW3D DATAIN SURF PAGEN ASEMBL BLKITR PRINTT' READR READN		I I I I I I I I I
LUPAR	--	Scalar	Logical Unit for Storing Binary Pointer Arrays	GW3D		I
LUSTO	--	Scalar	Logical Unit for Storing Binary Output	GW3D STORE		I I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MAXBES	--	Scalar	Maximum No. of Boundary Element Surfaces	STORE	SGEOM	I
MAXBNP	--	Scalar	Maximum No. of Boundary Nodal Points	PRINTT STORE	SGEOM	I I
MAXBw	--	Scalar	Maximum No. of Bandwidth	SOLVE		I
MAXEL	--	Scalar	Maximum No. of Elements	SPROP PRINTT STORE	SGEOM	I I I
MAXELK	--	Scalar	Maximum No. of Elements			
MAXM.AT	--	Scalar	Maximum No. of Materials	SPROP	SMTL	I
MAXNOD	--	Scalar	Maximum No. of Data Points to be Read	READR		I
MAXNP	--	Scalar	Maximum no. of Nodal Points	SPROP BLKITR SOLVE PRINTT STORE	SGEOM	I I I I I
MAXNPK	--	Scalar	Maximum No. of Nodes			
MAXNTI	--	Scalar	Maximum No. of Time Steps		SGEOM	
MXBESK	--	Scalar	Maximum No. of Boundary Element Surfaces			
MXBNPK	--	Scalar	Maximum No. of Boundary Nodal Points			
MXCDP	--	Scalar	Maximum No. of Data Points on Each Cauchy-Flux Profile		CCBC	
MXCDPK	--	Scalar	Maximum No. of Data Points on Each Cauchy-Flux Profile			
MXCES	--	Scalar	Maximum No. of Specified-Flux (Cauchy) Element Surfaces		CCBC	
MXCESK	--	Scalar	Maximum No. of Specified-Flux (Cauchy) Element Surfaces			
MXCNP	--	Scalar	Maximum No. of Specified-Flux (Cauchy) Nodal Points		CCBC	

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MXCNPK	--	Scalar	Maximum No. of Specified-Flux (Cauchy) Nodal Points			
MXCPR	--	Scalar	Maximum No. of Specified-Flux (Cauchy) Profiles		CCBC	
MXCPRK	--	Scalar	Maximum No. of Specified-Flux (Cauchy) Profiles			
MXDDP	--	Scalar	Maximum No. of Data Points on Each Dirichlet Profile		CDBC	
MXDDPK	--	Scalar	Maximum No. of Data Points on Each DirIchlet Profile			
MXDNP	--	Scalar	Maximum No. of Dirichlet Nodal Points		CDBC	
MXDNPK	--	Scalar	Maximum No. of Dirichlet Nodal Points			
MXDP	--	Scalar	Maximum No. of Data Points in any Profile	ALLFCT		I
MXDPR	--	Scalar	Maximum No. of Dirichlet Total Head Profiles		CDBC	
MXDPRK	--	Scalar	Maximum No. Dirichlet Total Head Profiles			
MXDTCK	--	Scalar	Maximum No. of DELT Changes			
MXJBD	--	Scalar	Maximum No. of Nonzero Elements in any Row	BLKITR PRINTT		I I
MXJBDK	--	Scalar	Maximum No. of Nonzero Elements in any Row			
MXMATK	--	Scalar	Maximum No. of Material Types			
MXMPMK	--	Scalar	Maximum No. of Material Properties per Material			
MXMPPM	--	Scalar	Maximum No. of Material Properties per Material		SMTL	
MXNDP	--	Scalar	Maximum No. of Data Points on Each Neumann-Flux Refile		CNBC	

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MXNDPK	--	Scalar	Maximum No. of Data Points on Each Neumann-Flux Profile			
MXNDTC	--	Scalar	Maximum No. of DELT Changes		SGEOM	
MXNES	--	Scalar	Maximum No. of Neumann Element Surfaces		CNBC	
MXNESK	--	Scalar	Maximum No. of Neumann Element Surfaces			
MXNNP	--	Scalar	Maximum No. of Neumann Nodal Points		CNBC	
MXNNPK	--	Scalar	Maximum No. of Neumann Nodal Points			
MXNPR	--	Scalar	Maximum No. of Neumann-Flux Profiles		CNBC	
MXNPRK	--	Scalar	Maximum No. of Neumann-Flux Profiles			
MXNTIK	--	Scalar	Maximum No. of Time Steps			
MXPR	--	Scalar	Maximum No. of Profiles	ALLFCT		I
MXRDP	--	Scalar	Maximum No. of Data Points on Each Rainfall Profile		CVBC	
MXREGN	--	Scalar	Maximum No. of Subregions	BLKITR STORE	LGEOM	I I
MXRGNK	--	Scalar	Maximum No. of Subregions			
MXRPR	--	Scalar	Maximum No. of Rainfall Profiles		CVBC	
MXSDP	--	Scalar	Maximum No. of Data Points on Each Element Soured Sink Profile		CS	
MXSDPK	--	Scalar	Maximum No. of Data Points on Each Element Source/ Sink Profile			
MXSEL	--	Scalar	Maximum No. of Source Elements		CS	

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARLABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MXSELK	--	Scalar	Maximum No. of Source Elements			
MXSPMK	--	Scalar	Maximum No. of Soil Parameters per Material to Describe Soil Characteristic Curves			
MXSPPM	--	Scalar	Maximum No. of Soil Parameter Per Material to Describe Soil Characteristic Curves	SPROP	SMTL	I
MXSPR	--	Scalar	Maximum No. of Source Profiles		CS	
MXSPRK	--	Scalar	Maximum No. of Source Profiles			
MXTYP	--	Scalar	Maximum No. of Integers Allowed to be Read	READN		I
MXVDPK	--	Scalar	Maximum No. of Data Points on Each Rainfall Profile			
MXVES	--	Scalar	Maximum No. of Variable Element Surfaces		CVBC	
MXVESK	--	Scalar	Maximum No. of Variable Element Surfaces			
MXVNP	--	Scalar	Maximum No. of Variable Nodal Points	PRINTT	CVBC	I
MXVNPK	--	Scalar	Maximum No. of Variable Nodal Points			
MXVPRK	--	Scalar	Maximum No. of Rainfall Profiles			
MXWDP	--	Scalar	Maximum No. of Data Points on Each Well Source/Sink Profile		CW	
MXWDPK	--	Scalar	Maximum No. of Data Points on Each Well Source/Sink Profile			
MXWNP	--	Scalar	Maximum No. of Well Nodal Points		CW	

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MXWNPK	--	Scalar	Maximum No. of Well Nodal Points			
MXWPR	--	Scalar	Maximum No. of Well Source/Sink Profiles		CW	
MXWPRK	--	Scalar	Maximum No. of Well Source/Sink Profiles			
N	--	Scalar	Base Functions Associated with 8 Nodes of the Element	BASE		O
NBES	--	Scalar	Number of Boundary Element Surfaces	STORE	CGEOM	I
NBNP	--	Scalar	Number of Boundary Nodal Points	STORE	CGEOM	I
NCDP	--	Scalar	Number of Data Points on Specified-Flux (Cauchy) Profiles		CCBC	
NCES	--	Scalar	Number of Specified-Flux (Cauchy) Boundary Element Sides		CCBC	
NCHG	--	Scalar	Number of Variable Boundary Nodes that has Changed Boundary Conditions	BCPREP		O
NCNP	--	Scalar	Number of Specified-Flux (Cauchy) Boundary Nodal Points		CW	
NCPR	--	Scalar	Number of Specified-Flux (Cauchy) Profiles		CCBC	
NCYL	--	Scalar	Number of Cycles per Time Step		CINTE	
NDDP	--	Scalar	Number of Data Points on Dirichlet Profiles		CDBC	
NDNP	--	Scalar	Number of Dirichlet Nodal Points		CDBC	
NDP	--	Scalar	Number of Data Points in Any Profile	ALLFCT		I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
NDPR	--	Scalar	Number of Dirichlet Profiles		CDBC	
NDTCHG	--	Scalar	Number of Times to Reset Time Step Size		CGEOM	
NEL	--	Scalar	Number of Elements	SPROP PRINTT STORE	CGEOM	
NITER	--	Scalar	Number of Iterations per Cycle	BLKXTR	CINTE	
NMAT	--	Scalar	Number of Materials		CMTL	
NMPPM	--	Scalar	Number of Material Properties per Material		CMTL	
NNDP	--	Scalar	Number of Data Points on Neumann-Flux Profiles		CNBC	
NNES	--	Scalar	Number of Neumann Boundary Element Sides		CNBC	
NNNP	--	Scalar	Number of Neumann Boundary Nodal Points		CNBC	
NNP	--	Scalar	Number of Nodal Points	BLKITR SOLVE PRINTT STORE READR	CGEOM	I I I I I
NNPLR(K)	--	Array	Number of Node Points in the K-th Subregion	GW3D DATAIN PAGEN BLKITR STORE		M O I I I
NNPR	--	Scalar	Number of Neumann-Flux Profiles		CNBC	
NPBB(I)	--	Array	Global Node Number of the I-th Boundary Node	GW3D DATAIN SURF SFLOW STORE		M O O I I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Block	I,M,O
NPCB(MP)	--	Array	Global Node Number of the MP-th Cauchy Node on Input, then is Changed to Contain the Boundary Node Number	GW3D DATAIN SFLOW		M O I
NPCNV(I)	--	Array	Global Node Number of the I-th Nonconvergent Node	GW3D		M
NPCON(NP)	--	Array	Pending Condition Indicator of the NP-th VB Node: O = this is not a Pondidng-Condition Node for the Present Time Step, Global Node Number = this is a Ponding-Condition Node for the Present Time	GW3D BCPREP BC PRINTT		M O I I
NPDB(MXDNP)	--	Array	Global Node Number of the NP-th Dirichlet Node	GW3D DATAIN BC SFLOW		M O I I
NPFLX(NP)	--	Array	Flux Boundary Condition Indicator of the NP-th VB Node; O = this is not a Flux-Condition Node for the Present Time Step, Global Node Number = This is a Flux-Condition Node for the Present Time	GW3D BCPREP BC PRINTT		M O I I
NPITER	--	Scalar	Number of Blockwise Iterations Allowed		CINTE	
NPMIN(NP)	--	Array	Minimum-Pressure Condition Indicator of the NP-th VB Node; O = this is not a Minimum-Pressure-Condition	GW3D BCPREP BC PRINTT		M O I I
NPNB(MP)	--	Array	Global Node Number of the MP-th Neumann Node on Input, then is Changed to Contain the Boundary Node Number	GW3D DATA-IN SFLOW		M O I
NPR	--	Scalar	Number of Profiles	ALLFCT		I
NPROB	--	Scalar	Problem Number	STORE		I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NPVB(NP)	--	Array	Global Node Number of the NP-th VB Node on Input, then is Changed to Contain the Boundary Node Number	GW3D DATAIN SFLOW PRINTT		M O I I
NPW(NP)	--	Array	Global Node Number of the NP-th S/S Well Node	GW3D DATAIN ASEMBL		M O I
NRDP	--	Scalar	Number of Data Points on Rainfall Profiles		CVBC	
NREGN	--	Scalar	Number of Subregions	BLKITR STORE	LGEOM	I I
NRPR	--	Scalar	Number of Rainfall Profiles		CVBC	
NSDP	--	Scalar	Number of Data Points on Element-Source/Sink Profile		CS	
NSEL	--	Scalar	Number of Element-Source/ Sink and B.C. Control Integer		CS	
NSPPM	--	Scalar	Number of Soil Parameters per Material to Describe Soil Characteristic Curves	SPROP	CMTL	
NSPR	--	Scalar	Number of Element-Source/ Sink Profiles		CS	
NTI	--	Scalar	Number of Time Increments	STORE	CGEOM	I
NTNPLR(K)	--	Array	Total Number of Nodes for the K-th Subregion Including Interior, Global Boundary, and Intra-boundary Nodes	GW3D PAGEN DATAIN		M O O
NTYPE	--	Scalar	Number of Integers to be Read	READN		I
NVES	--	Scalar	Number of Variable Bounda~ Element Sides	CVBC		
NVNP	--	Scalar	Number of Variable Boundary Nodal Points	PRINTT	CVBC	

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NWDP	--	Scalar	Number of Data Points on Each Well Source/Sink Profile		CW	
NWNP	--	Scalar	Number of Well Source/Sink Nodal Points		CW	
NWPR	--	Scalar	Number of Well Source/Sink Profiles		CW	
OME	--	Scalar	Iteration Parameter for a Non-Linear Equation	BLKITR	CREAL	I
OMI	--	Scalar	Relaxation Parameter for Pointwise Solution		CREAL	
PR(MXPR)	L or L^3/L^2	Array	Profile Values at T	ALLFCT		O
PRF(MXDP, MXPR)	L or L^3/L^2	Array	Profile Value of the Data Point on the Profile	ALLFCT		I
PROP(I,J)	L/T or L'	Array	I-th Material Property of the J-th Material; I = 1 = saturated xx-hydraulic conductivity 1 = 2 = saturated yy-hydraulic conductivity 1 = 3 = saturated zz-hydraulic conductivity 1 = 4 = saturated xy-hydraulic conductivity 1 = 5 = saturated xz-hydraulic conductivity 1 = 6 = saturated yz-hydraulic conductivity	GW3D DATAIN VELT ASEMBL BC		M O I I I
QA(8,8)	--	Array	Integration of N(I) *DTH/DH*N(J)	Q8		O
QB(8,8)	--	Array	8 x 8 Element Matrix	Q8DV Q8		O O

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
QCB(J)	$L^3/T/L^2$	Array	Cauchy Flux of the J-th Profile at the Present Time	GW3D BC		M I
QCBF(I,J)	$L^3/T/L^2$	Array	Cauchy Flux of the I-th Data Point in the J-th Profile	GW3D DATAIN		M O
QNB(J)	$(L^3/T)/L^2$	Array	Neumann Flux of the J-th Profile at the Present Time	GW3D BC		M I
QNBF(I,J)	L'/T/L'	Array	Neumann Flux of the I-th Data Point in the J-th Profile	GW3D DATAIN		M O
QRX(8)	--	Array	X-Velocity Element Vector	Q8DV		O
QRY(8)	--	Array	Y-Velocity Element Vector	Q8DV		O
QRZ(8)	--	Array	Z-Velocity Element Vector	Q8DV		O
QSOSM	L^3	Scalar	Integration of SOURCE	Q8TH		O
QTHM	L^3	Scalar	Integration of DHQ*THG	Q8TH		O
R(MAXNP)	--	Array	Load Vector	SOLVE		M
RF(I,J)	L/T	Array	Rainfall Rate of I-th Data Point in J-th Profile	GW3D DATAIN		M O
RFALL(JJ)	L/T'	Array	Rainfall Rate of J-th Profile at the Present Time	GW3D BCPREP		M I
RI(N)	L	Array	Pressure Head Iterate in BLKITR	GW3D		M
RL	--	Scalar	A Working Array to Contain the Final Solution of the Pressure Head in BLKITR	GW3D		M
RLD(N)	--	Array	An Array to Store the Assembled Global Load Vector	GW3D ASEMBL BC		M O M
RLDG(MAXNP)	--	Array	Global Load Vector	BLKITR		I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
RLDL(N)	--	Array	Assembled Load Vector for a Subregion	GW3D BLKITR		M M
RQ(8)	--	Array	Integration of N(I).K. (Unit Vector in Z)	Q8		O
R1Q(4)	--	Array	Integration of N(I)*F1Q Over the Boundary Segment	Q4S		O
R2Q(4)	--	Array	Integration of N(I)*F2Q Over the Boundary Segment	Q4S		O
SOS(J)	$(L^3/T)/L^3$	Array	Value of J-th Element Source/Sink at Present Time	GW3D ASEMBL SFLOW		M I I
SOSF(I,J)	$L^a/'l'/L^2/L$	Array	S/S Rate of the I-th Data Point in the J-th Profile	GW3D DATAIN		M O
SOSM	L^3/T	Scalar	Source/Sink Strength of the Element	Q8		I
SOURCE	L^3/T	Scalar	Element Source/Sink Strength	Q8TH		I
SS	--	Scalar	Xsi-Coordinate of the Gaussian Point	BASE		I
SUBHD	--	Char.	Subheading	PRINTT		I
T	T	Scalar	Time	ALLFCT		I
TDTCH(I)	T	Array	Time of the I-th Time to Reset the Time Step Size to Initial Time Step Size	GW3D DATAIN		M O
TFLOW(10)	L^3	Array	Total Flow		CFLOW	
TH(I,M)	--	Array	Moisture Content, at the I-th Node of the M-th Element	GW3D SPROP SFLOW PRINTT STORE		M O I I I
THDBF(I,J)	T	Array	Time of the I-th Data Point in J-th Head Profile	GW3D DATAIN		M O
THG(8)	--	Array	Moisture Content at Eight Gaussian Points of the Element	Q8TH		I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
THPROP (I,J)	--	Array	I-th Parameter to Describe the Moisture Content as a Function of Pressure Head for the J-th Material or I-th Data Point of Moisture Content for the J-th Material	GW3D DATAIN SPROP		M O I
TIME	T	Scalar	Real Simulation Time	PRINTT STORE		
TITLE	--	Char.	Title of the Problem	STORE		
TMAX	T	Scalar	Maximum Value of Time		CREAL	
TOLA	L	Scalar	Steady-State Tolerance		CREAL	
TOLB	L	Scalar	Transient State Tolerance	BLKITR	CREAL	
TPRF(MXDP, MXPR)	T	Array	Time of the Data Point on the Profile	ALLFCT		
TQCBF(I,J)	T	Array	Time of the I-th Data Point in the J-th Specified-Flux (Cauchy) Profile	GW3D DATAIN		M O
TQNBF(I,J)	T	Array	Time of the I-th Data Point in the J-th Neumann Profile	GW3D DATAIN		M O
TRF(I,J)	T	Array	Time of the I-th Date Point in J-th Rainfall Profile	GW3D DATAIN		M O
TSOSF(I,J)	T	Array	Time of the I-th Data Point in the J-th Profile	GW3D DATAIN		M O
TT	--	Scalar	Eta-Coordinate of the Gaussian Point	BASE		I
TWSSF(I,J)	T	Array	Time of the I-th Data Point in the J-th Profile	GW3D DATAIN		M O
UU	--	Scalar	Zeta-Coordinate of the Gaussian Point	BASE		I
VX(N)	L/T	Array	X-Component Velocity at the N-th Node	GW3D VELT BCPREP		O O I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
				SFLOW		I
				PRINTT		I
				STORE		I
VY(N)	L/T	Array	Y-Component Velocity at the N-th Node	GW3D		O
				VELT		O
				BCPREP		I
				SFLOW		I
				PRINTT		I
				STORE		I
VZ(N)	UT	Array	Z-Component Velocity at the N-th Node	GW3D		O
				VELT		O
				BCPREP		I
				SFLOW		I
				PRINTT		I
				STORE		I
W(8)	--	Array	Weighting Function at Eight Points of the Element	ASEMBL	CREAL	I
WSS(J)	L^3/T	Array	Value of the J-th Well Source/Sink at Present Time	GW3D		M
				SFLOW		I
				ASEMBL		I
WSSF(I,J)	L^3/T	Array	S/S Rate of the I-th Data Point in the J-th Profile	GW3D		M
				DATAIN		O
X(N)	L	Array	X-Coordinate of the N-th Node	GW3D		M
				DATAIN		O
				SURF		I
				VELT		I
				BCPREP		I
				ASEMBL		I
				BC		I
				SFLOW		I
				STORE		I
XQ(8)	L	Array	X-Coordinate at Eight Nodes of the Element	Q8DV		I
				Q8		I
				BASE		I
				Q4S		I
				Q8TH		I

TABLE D-1. 3DFEMWATER PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
Y(N)	L	Array	Y-Coordinate of the N-th Node	GW3D		M
				DATAIN		O
				SURF		I
				VELT		I
				BCPREP		I
				ASEMBL		I
				BC		I
				SFLOW		I
				STORE		I
YQ(8)	L	Array	Y-Coordinate at Eight Nodes of the Element	Q8DV		I
				Q8		I
				BASE		I
				Q4S		I
				Q8TH		I
Z(N)	L	Array	Z-Coordinate of the N-th Node	GW3D		M
				DATAIN		O
				SURF		I
				VELT		I
				BCPREP		I
				ASEMBL		I
				BC		I
				SFLOW		I
				STORE		I
ZQ(8)	L	Array	Z-Coordinate at Eight Nodes of the Element	Q8DV		I
				Q8		I
				BASE		I
				Q4S		I
				Q8TH		I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION

Variable	Unite	Type	Description	Sub-routine	Common Block	I,M,O
AL	L	Scalar	Longitudinal Dispersivity	Q8DV Q8		I I
AM	L'/'I'	Scalar	Modecular Diffusion Coefficient	Q8		I
APHA1	--	Scalar	Weighting Factor for Side 1-2 Parallel to the X-direction		WETX	
APHA2	--	Scalar	Weighting Factor for Side 4-3 Parallel to the X-direction		WETX	
APHA3	--	Scalar	Weighting Factor for Side 5-6 Parallel to the X-direction		WETX	
APHA4	--	Scalar	Weighting Factor for Side 8-7 Parallel to the X-direction		WETX	
AT	L	Scalar	Lateral Dispersivity	Q8DV Q8		I I
BETAl	--	Scalar	Weighting Factor for Side 1-4 Parallel to the Y-direction		WETY	
BETA2	--	Scalar	Weighting Factor for Side 2-3 Parallel to the Y-direction		WETY	
BETA3	--	Scalar	Weighting Factor for Side 5-8 Parallel to the Y-direction		WETY	
BETA4	--	Scalar	Weighting Factor for Side 6-7 Parallel to the Y-direction		WETY	
BFLX(I)	M/T	Array	Boundary Flux at the I-th Boundary Node	GM3D SFLOW		M M
BFLXP(I)	M/T	Array	Value of BFI.X(I) at the Previous Time	GM3D SFLOW		M M
BQ(4,4)	--	Array	A 2 by 2 Boundary Surface Matrix	Q4CNVB		O

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
C(N)	M/L³	Array	Concentration of the N-th Node at the Present Time	GM3D FLUX BLKITR SOLVE SFLOW PRINTT STORE		O I O M I I I
CDB(I)	M/L³	Array	Dirichlet Concentration of the I-th Profile at Present Time	GM3D BC ADVBC		M I I
CDBF(I,J)	M/L³	Array	Concentration of the I-th Data Point in the J-th Dirichlet Concentration vs. Time Profile	GM3D DATAIN		M M
CHNG	--	Scalar	Multiplier for Increasing DELT		CREAL	
CMATRX (N,I)	--	Array	An Array to Store the I-th Non-Zero Entry of the N-th Equation of the Assembled Global Matrix	GM3D FLUX ASEMBL BC		M O O O
CMTRXG (N,I)	--	Array	Global Matrix	BLKITR		I
CMTRXL (N,I)	--	Array	Assembled Matrix for a Subregion	GM3D BLKITR		M I
CP(N)	M/L³	Array	Concentration of the N-th Node at the Previous Time	GM3D DATAIN ASEMBL ADVTRN		O M I I
CQ(8)	M/L³	Array	Dissolved Concentration at Eight Points of an Element	Q8DV Q8R		I I
CSQ(8)	M/M	Array	Adsorbed Concentration at Eight Points of an Element	Q8R		I
CSTAR(N)	M/L³	Array	Lagrangian Concentration at the N-th Node	GM3D ASEMBL ADVTRN ADVBC		O I O O

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
CVB(I)	M/L³	Array	Variable Concentration of the I-th Profile at the Present Time	GM3D BC ADVBC		M I I
CVBF(I,J)	M/L³	Array	Concentration of the I-th Data Point in the J-th Variable Concentration vs. Time Profile	GM3D DATAIN		M M
CW(N)	M/L³	Array	Nonlinear Iterate of the Concentration at the N-th Node	GM3D ASEMBL		O I
CWQ(8)	M/L³	Array	Iterate of the Dissolved Concentration at Eight Gaussian Points of the Element	Q8		I
DCOSB(l,I)	--	Array	X-Directional Cosine of the I-th Boundary Side	GM3D DATAIN SURF BC Q4CNVB SFLOW ADVBC Q4ADB		M M O I I I I I
DCOSB(2,1)	--	Array	Y-Directional Cosine of the I-th Boundary Side	GM3D DATAIN SURF BC Q4CNVB SFLOW ADVBC Q4ADB		M M O I I I I I
DCOSB(3,1)	--	Array	Z-Directional Cosine of the I-th Boundary Side	GM3D DATAIN SURF BC Q4CNVB SFLOW ADVBC Q4ADB		M M O I I I I I
DD	L'PI!	Scalar	Effective Molecular Diffusion Coefficient	Q8DV		I
DELMAX	T	Scalar	Maximum Value of DELT		CREAL	

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
DELT	T	Scalar	Time Increment	ASEMBL SFLOW PRINTT' NDTAU	CREAL	I I I I
DELTO	T	Scalar	Time Increment		CREAL	
DJAC	L^3	Scalar	Determinant of the Jacobian	SHAPE		O
DNX(8)	1/L	Array	Partial Derivative of the Base Function with Respect to x	SHAPE		O
DNY(8)	1/L	Array	Partial Derivative of the Base Function with Respect to Y	SHAPE		O
DNZ(8)	1/L	Array	Partial Dervative of the Base Function wtih Respect to z	SHAPE		O
DSDCQ(8)	$L^3$1M	Array	The Derivative of Adsorbed Concentration with Respect to Dissolved Concentration at Eight Points of the Element	Q8		
DTAU	T	Scalar	Sub-Time Step Size	NDTAU ADVTRN		O I
DTH(I,M)	1/L	Array	(TH(I,M)-THP(I,M)/DELT	GM3D ASEMBL		M I
DTHG(8)	1/T	Array	dTH/dt at Eight Gaussian Points of the Element	Q8		I
ETA	--	Scalar	Local Coordinate of the Particle	XSI3D		O
F(MAXNOD)	--	Array	Array of Real Numbers that are to be Read and Generated Automatically	READR		O
FLOW	M/L	Scalar	Increment of Flow		CFLOW	
FQ(d)	$M/L^2/T$	Array	Normal Flux at Four Points of the Element Surface	Q4BB		I
FRATE	M/T	Scalar	Flow Rate		CFLOW	

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
FX(N)	$(M/L^2)/T$	Array	X-Direction Material Flux at the N-th Node	GM3D FLUX SFLOW PRINTT STORE		O O I I I
N(N)	$M/L^2/T$	Array	Y-Direction Material Flux at the N-th Node	GM3D FLUX SFLOW PRINTT STORE		O O I I I
FZ(N)	$M/L^2/T$	Array	Z-Direction Material Flux at the N-th Node	GM3D FLUX SFLOW PRINTT STORE		O O I I I
GAMA1	--	Scalar	Weighting Factor for Side 1-5 Parallel to the Z-direction		WETZ	
GAMA2	--	Scalar	Weighting Factor for Side 2-6 Parallel to the Z-direction		WETZ	
GAMA3	--	Scalar	Weighting Factor for Side 4-8 Parallel to the Z-direction		WETZ	
GAMA4	--	Scalar	Weighting Factor for Side 3-7 Parallel to the Z-direction		WETZ	
GNLR(I,K)	--	Array	Global Nodal Number of the I-th Local Nodal Number in the K-th Sub-region. This Array is an Input for I = 1, 2, .., NNPLR(K). For I = NNPLR(K)+l, . . . NTNPLR(K), this Array is Generated Based on IE(NEL,8) and Inputted GNLR.	GM3D DATAIN PAGEN BLKITR		M M M I
IBC	--	Scalar	Index of Boundary Condition Type	Q4CNVB Q4ADB		

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Block	I,M,O
IBUG	--	Scalar	Debugging Indicator	BLKITR		
IICTYP(MP)	--	Array	Type of Specified-Flux (Cauchy) Profile Assigned to the MP-th Cauchy Side	GM3D		M
				DATAIN		M
				BC		I
				ADVBC		I
IDTYP(NP)	--	Array	Type of Dirichlet Concentration Profile Assigned to the NP-th Dirichlet Node	GM3D		M
				DATAIN		M
				BC		I
				ADVBC		I
IE(M,I)	--	Array	Global Node Number of the I-th Node of the M-th Element if I is Between 1 and 8. When I = 9, This is an Integer to Indicate the Material Type of the M-th Element.	GM3D		M
				DATAIN		M
				SURF		I
				PAGEN		I
				LELGEN		I
				AFABTA		I
				ASEMBL		I
				BC		I
				FLUX		I
				SFLOW		I
				STORE		I
				THNODE		I
				NDTAU		I
				ADVTRN		I
				MPLOC		I
				ADVBC		I
IGEOM	--	Scalar	Geometry Description Output Control	LELGEN	CINTE	I
IHALFB	--	Scalar	Half Band Width Plus 1	SOLVE		I
ILUMP	--	Scalar	Lumping Indicator		OPTN	
INDTYP(MXTYP)	--	Array	Army of Integers that are to be Read or Generated Automatically	READN		O
INTYP(MP)	--	Array	Type of Specified-Dispersive-Flux (Neumann) Profile Assigned to the MP-th Neumam Side	GM3D		M
				DATAIN		M
				BC		I
IOPTIM	--	Scalar	Optimizing Weighting Factor Indicator	AFABTA	OPTN	I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ISB(l,I)	--	Array	Boundary Node Number of the First Node of the I-th Boundary Side	GM3D		M
				DATAIN		M
				SURF		O
				BC		I
				SFLOW		I
				ADVBC		I
ISB(2,I)	--	Array	Boundary Node Number of the Second Node of the I-th Boundary Side	GM3D		M
				DATAIN		M
				SURF		O
				BC		I
				SFLOW		I
				ADVBC		I
ISB(3,I)	--	Array	Boundary Node Number of the Third Node of the I-th Boundary Side	GM3D		M
				DATAIN		M
				SURF		O
				BC		I
				SFLOW		I
				ADVBC		I
ISB(4,I)	--	Array	Boundary Node Number of the Fourth Node of the I-th Boundary Side	GM3D		M
				DATAIN		M
				SURF		O
				BC		I
				SFLOW		I
				ADVBC		I
ISB(5,I)	--	Array	Element Side Index of the I-th Boundary Side: l=left side, 2=front side, 3=right side, 4=back side, 5=bottom side, 6=top side	GM3D		M
				DATAIN		M
				SURF		O
				BC		I
				SFLOW		I
				ADVBC		I
ISB(6,I)	--	Array	Element Number to which the I-th Boundary Side Belongs	GM3D		M
				DATAIN		M
				SURF		O
				BC		I
				SFLOW		I
				ADVBC		I
ISC(l,MP)	--	Array	Global Node Number of the First Node of the MP-th Specified-Flux (Cauchy) Side	GM3D		M
				DATAIN		M
				BC		I
				ADVBC		I
ISC(2,MP)	--	Array	Global Node Number of the Second Node of the MP-th Specified-Flux (Cauchy) Side	GM3D		M
				DATAIN		M
				BC		I
				ADVBC		I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ISC(3,MP)	--	Array	Global Node Number of the Third Node of the MP-th Specified-Flux (Cauchy) Side	GM3D DATAIN BC ADVBC		M M I I
ISC(4,MP)	--	Array	Global Node Number of the Fourth Node of the MP-th Specified-Flux (Cauchy) Side	GM3D DATAIN BC ADVBC		M M I I
ISC(5,MP)	--	Array	Boundary Side Number of the MP-th Specified-Flux (Cauchy) Side	GM3D DATAIN BC ADVBC		M M I I
ISN(l,MP)	--	Array	Global Node Number of the First Node of the MP-th Specified-Dispersive-Flux (Neumann) Side	GM3D DATAIN BC		M M I
ISN(2,MP)	--	Array	Global Node Number of the Second Node of the MP-th Specified-Dispersive-Flux (Neumann) Side	GM3D DATAIN BC		M M I
ISN(3,MP)	--	Array	Global Node Number of the Third Node of the MP-th Specified-Dispersive-Flux (Neumann) Side	GM3D DATAIN BC		M M I
ISN(4,MP)	--	Array	Global Node Number of the Fourth Node of the MP-th Specified-Dispersive-Flux (Neumann) Side	GM3D DATAIN BC		M M I
ISN(5,MP)	--	Array	Boundary Side Number of the MP-th Neumann Side	GM3D DATAIN BC		M M I
ISTYP(M)	--	Array	Type of Source Profile Assigned to the M-th Element	(IM3D DATAIN ASEMBL SFLOW		M M I I
ISV(l,MP)	--	Array	Global Node Number of the First Node of the MP-th Variable Side	GM3D DATAIN BC ADVBC		M M I I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ISV(2,MP)	--	Array	Global Node Number of the Second Node of the MP-th Variable Side	GM3D DATAIN BC ADVBC		M M I I
ISV(3,MP)	--	Array	Global Node Number of the Third Node of the MP-th Variable Side	GM3D DATAIN BC ADVBC		M M I I
ISV(4,MP)	--	Array	Global Node Number of the Fourth Node of the MP-th Variable Side	GM3D DATAIN BC ADVBC		M M I I
ISV(5,MP)	--	Array	Boundary Side Number of the MP-th Variable Side	GM3D DATAIN BC ADVBC		M M I I
ITIM	--	Scalar	Time-Step Index	PRINTT		I
IVTYP(MP)	--	Array	Type of Variable Concentration Profile Assigned to the MP-th Variable Side	GM3D DATAIN BC ADVBC		M M I I
IWET	--	Scalar	Upstream Weighting Indicator		OPTN	
IWTYP(I)	--	Array	Type of Source Profile Assigned to the I-th Node	GM3D DATAIN ASEMBL SFLOW		M M I I
KANALY	--	Scalar	Analytical Input Control	ALLFCT		I
KCAI	--	Scalar	Analytical Cauchy-Flux Input Control		CCBC	
KDAl	--	Scalar	Analytical Dirichlet Input Control		CDBC	
KDIAG	--	Scalar	Diagnostic Output Table Index	PRINTT		O
KDSK(I)	--	Array	Store Results on Logical Unit 12 for the I-th Time Step? 0=no, l=yes	GM3D DATAIN		M M
KDSKO	--	Scalar	Disk Output Control		CINTE	

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
3KFLOW	--	Scalar	Flow Indicator -1 = Initial or Pre-initial Condition O = Steady-state 1. Transient	SFLOW		I
KKK	--	Scalar	Decomposition or Back Substitution Indicator 1 = Decomposition 2 = Back Substitution	SOLVE		I
KNAI	-	Scalar	Analytical Neumann Flux Input Control		CNBC	
KOUT	--	Scalar	Output-Table Number Index	PRINTT		O
KPR(I)	--	Array	Line Printing Indicator for the I-th Time Step: O = print nothing 1 = print fluxes through all types of boundaries 2 = print concentration also 3 = print material flux also	GM3D DATAIN BLKITR PRINTT		M M I I
KPRO	--	Scalar	Output Control		CINTE	
KRAI	--	Scalar	Analytical Rainfall Input Control		CVBC	
KSAI	--	Scalar	Elemen-source Input Control		CELS	
KSORP	--	Scalar	Sorption Model Indicator	THNODE	OPTN	I
KSS	--	Scalar	Steady-State I.C. Control	ASEMBL	CINTE	I
KVI	--	Scalar	Flow Variable Input Control		CINTE	
KWAI	--	Scalar	Well Source Input Control O = Tabular Input 1 = Analytical Input		CNPS	
LAMBDA	1/T	Scalar	Decay Constant	Q8		I
LES(I)	---	Array	Global Element Number of the I-th Element-Source	GM3D DATAIN ASEMBL SFLOW		M M I I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
LMAXDF(K)	--	Array	Maximum No. of Difference Between Nodes for Any Element in the K-th Local Region. This Array is Generated from the Array LNOJCN.	GM3D PAGEN BLKITR DATAIN		M O I M
LMXBW	--	Scalar	Maximum No. of the Band-width in Any Subregion		LGEOM	
LMXBWK	--	Scalar	Maximum No. of the Band-width in Any Subregion			
LMXNP	--	Scalar	Maximum No. of Nodal Points in Any Subregion, Including Interior Nodes and Global Boundary Nodes		LGEOM	
LMXNPK	--	Scalar	Maximum No. of Nodal Points in Any Subregion, Including Interior Nodes and Global Boundary Nodes			
LNOJCN(J, I,K)	--	Array	Local Node Number of the J-th Node Connecting to I-th Local Node for the K-th Subregion. This Array is Generated from GNLR and 1 =1,2,3, . . . , NNPLR(K).	GM3D PAGEN BLKITR DATAIN		M O I M
LOCP	--	Scalar	Indicator of the Location of the Fictitious Particle	MPLOC		O
LRM(I,N)	--	Array	Global Element Number of the I-th Element Connect ing to the N-th Global Node	GM3D LELGEN NDTAU ADVTRN MPLOC DATAIN PAGEN SURF		M O I I I M O I
LRN(I,N)	--	Array	Global Node Number of the I-th Node Connecting to the N-th Global Node	GM3D PAGEN ASEMBL BC NDTAU DATAIN		M O I I I M

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
LTMXNK	--	Scalar	Maximum No. of Total Nodal Points in Any Subregion, Including Interior Nodes, and Global Boundary Nodes			
LTMXNP	--	Scalar	Maximum No. of Total Nodal Points in Any Subregion, Including Interior Nodes, and Global Boundary Nodes		LGEOM	
LUBAR	--	Scalar	Logical Unit for Storing Binary Boundary Arrays	GM3D DATAIN		I I
LUFLW	--	Scalar	Logical Unit for Flow Data	GM3D DATAIN		I I
LUINP	--	Scalar	Logical Unit for Input Data	GM3D DATAIN READR READN		I I I I
LUOUT	--	Scalar	Logical Unit for Output Data	GM3D DATAIN SURF PAGEN LELGEN ASEMBL BLKITR PRINTT READR READN NDTAU ADVTRN XS13D BC		I I I I I I I I I I I I I I
LUPAR	--	Scalar	Logical Unit for Storing Binary Pointer Arrays	GM3D		I
LUSTO	--	Scalar	Logical Unit for Storing Binary Output	GM3D STORE		I I
M	--	Scalar	Element Number where the Fictitious Particle is Located	XS13D		I
MAXBES	--	Scalar	Maximum No. of Boundary Element Surfaces		SGEOM	
MAXBNP	--	Scalar	Maximum No. of Boundary Nodal Points		SGEOM	

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MAXBW	--	Scalar	Maximum No. of Band Width	SOLVE		I
MAXEL	--	Scalar	Maximum No. of Elements		SGEOM	
MAXELK	--	Scalar	Maximum No. of Elements			
MAXMAT	--	Scalar	Maximum No. of Materials		MATL	
MAXNOD	--	Scalar	Maximum No. of Data Points to be Read	READR		I
MAXNP	--	Scalar	Maximum No. of Nodal Points	SOLVE FCOS	SGEOM	I I
MAXNPK	--	Scalar	Maximum No. of Nodes			
MP	--	Scalar	Element where the Fictitious Particle is Located	MPLOC		O
MXBESK	--	Scalar	Maximum No. of Boundary-Element Surfaces			
MXBNPK	--	Scalar	Maximum No. of Boundary Nodal Points			
MXCDP	--	Scalar	Maximum No. of Data Points on Each Specified-Flux (Cauchy) Profile		CCBC	
MXCDPK	--	Scalar	Maximum No. of Data Points on Each Specified-Flux (Cauchy) Profile			
MXCES	--	Scalar	Maximum No. of Cauchy Element Surfaces		CCBC	
MXCESK	--	Scalar	Maximum No. of Cauchy Element Surfaces			
MXCNP	--	Scalar	Maximum No. of Cauchy Nodal Points		CCBC	
MXCNPK	--	Scalar	Maximum No. of Cauchy Nodal Points			
MXCPR	--	Scalar	Maximum No. of Cauchy-Flux Profiles		CCBC	

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MXCPRK	--	Scalar	Maximum No. of Cauchy-Flux Profiles			
MXDDP	--	Scalar	Maximum No. of Data Points on Each Dirichlet Profile		CDBC	
MXDDPK	--	Scalar	Maximum No. of Data Points on Each Dirichlet Profile			
MXDNP	--	Scalar	Maximum No. of Dirichlet Nodal Points		CDBC	
MXDNPK	--	Scalar	Maximum No. of Dirichlet Nodal Points			
MXDP	--	Scalar	Maximum No. of Data Points in Any Profile	ALLFCT		I
MXDPR	--	Scalar	Maximum No. of Dirichlet Total Head Profiles		CDBC	
MXDPRK	--	Scalar	Maximum No. of Dirichlet Total Head Profiles			
MXDTC	--	Scalar	Maximum No. of DELT Changes		SGEOM	
MXDTCK	--	Scalar	Maximum No. of DELT Changes			
MXJBD	--	Scalar	Maximum No. of Nonzero Elements in Any Row		SGEOM	
MXJBDK	--	Scalar	Maximum No. of Nonzero Elements in Any Row			
MXKBD	--	Scalar	Maximum No. of Elements Surrounding a Global Node		SGEOM	
MXKBDK	--	Scalar	Maximum No. of Elements Surrounding a Global Node			
MXMATK	--	Scalar	Maximum No. of Material Types			
MXMPMK	--	Scalar	Maximum No. of Material Properties per Material			
MXMPPM	--	Scalar	Maximum No. of Material Properties per Material		MATL	

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MXNDP	--	Scalar	Maximum No. of Data Points on Each Specified Dispersive-Flux (Neumann) Profile		CNBC	
MXNDPK	--	Scalar	Maximum No. of Data Points on Each Neumann-Flux Profile			
MXNES	--	Scalar	Maximum No. of Neumann Element Surfaces		CNBC	
MXNESK	--	Scalar	Maximum No. of Neumann Element Surfaces			
MXNNP	--	Scalar	Maximum No. of Neumann Nodal Points		CNBC	
MXNNPK	--	Scalar	Maximum No. of Neumann Nodal Points			
MXNPR	--	Scalar	Maximum No. of Neumann-Flux Profiles		CNBC	
MXNPRK	--	Scalar	Maximum No. of Neumann-Flux Profiles			
MXNTI	--	Scalar	Maximum No. of Time Steps		SGEOM	
MXNTIK	--	Scalar	Maximum No. of Time Steps			
MXPR	--	Scalar	Maximum No. of Profiles	ALLFCT		I
MXRDP	--	Scalar	Maximum No. of Data Points on Each Rainfall Profile		CVBC	
MXREGN	--	Scalar	Maximum No. of Subregions		LGEOM	
MXRGNK	--	Scalar	Maximum No. of Subregions			
MXRPR	--	Scalar	Maximum No. of Rainfall Profiles		CVBC	
MXSDP	--	Scalar	Maximum No. of Data Points in Any Element Source/Sink Profile		CELS	
MXSDPK	--	Scalar	Maximum No. of Data Points in Any Element Source/ Sink Profile			

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MXSEL	--	Scalar	Maximum No. of Source Elements		CELS	
MXSELK	--	Scalar	Maximum No. of Source Elements			
MXSPR	--	Scalar	Maximum No. of Element Source Profiles		CELS	
MXSPRK	--	Scalar	Maximum No. of Element Source Profiles			
MXTYP	--	Scalar	Maximum No. of Integers Allowed to be Read	READN		I
MXVDPK	--	Scalar	Maximum No. of Data Points on Each Rainfall Profile			
MXVES	--	Scalar	Maximum No. of Variable Element Surfaces		CVBC	
MXVESK	--	Scalar	Maximum No. of Variable Element Surfaces			
MXVNP	--	Scalar	Maximum No. of Variable Nodal Points		CVBC	
MXVNPK	--	Scalar	Maximum No. of Variable Nodal Points			
MXVPRK	--	Scalar	Maximum No. of Rainfall Profiles			
MXWDP	--	Scalar	Maximum No. of Data Points on Each Well Source/Sink Profile		CNPS	
MXWDPK	--	Scalar	Maximum No. of Data Points on Each Well Source/Sink Profile			
MXWNP	--	Scalar	Maximum No. of Well Nodal Points		CNPS	
MXWNPK	--	Scalar	Maximum No. of Well Nodal Points			
MXWPR	--	Scalar	Maximum No. of Well Source/Sink Profile		CNPS	

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MXWPRK	--	Scalar	Maximum No. of Well Source/Sink Profiles			
N(8)	--	Array	Base Function of Eight Points of the Element	SHAPE		O
NBES	--	Scalar	Number of Boundary Element Surfaces		CGEOM	
NBNP	--	Scalar	Number of Boundary Nodal Points		CGEOM	
NCDP	--	Scalar	Number of Data Points on Specified-Flux (Cauchy) Profiles		CCBC	
NCES	--	Scalar	Number of Cauchy Boundary Element Sides		CCBC	
NCM	--	Scalar	Number of. Cycles per Time step		CINTE	
NCNP	--	Scalar	Number of Cauchy Boundary Nodal Points		CCBC	
NCPR	--	Scalar	Number of Specified-Flux (Cauchy) Profiles		CCBC	
NDDP	--	Scalar	Number of Data Points on Dirichlet Profiles		CDBC	
NDNP	--	Scalar	Number of Dirichlet Nodal Points		CDBC	
NDP	--	Scalar	Number of Data Points in Any Profile	ALLFCT		I
NDPR	--	Scalar	Number of Dirichlet Profiles		CDBC	
NDTCHG	--	Scalar	Number of Times to Reset Time Step Size		CGEOM	
NEL	--	Scalar	Number of Elements		CGEOM	
NITER	--	Scalar	Number of Iterations per Cycle	BLKITR	CINTE	I
NMAT	--	Scalar	Number of Materials		MATL	

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NMPPM	--	Scalar	Number of Material Properties per Material		MATL	
NNDP	--	Scalar	Number of Data Points on Specified-Dispersive-Flux (Neumann) Profiles		CNBC	
NNES	--	Scalar	Number of Neumann Boundary Element Sides		CNBC	
NNNP	--	Scalar	Number of Neumann Boundary Nodal Points		CNBC	
NNP	--	Scalar	Number of Nodal Points	SOLVE READR	CGEOM	I I
NNPLR(K)	--	Array	Number of Nodes for the K-th Subregion Including Interior and Global Boundary Nodes	GM3D DATAIN PAGEN BLKITR		**M** **M** I I
NNPR	--	Scalar	Number of Specified-Dispersive-Flux (Neumann) Profiles		CNBC	
NODENP	--	Scalar	Nodal Point of Interest	MPLOC		I
NP1	--	Scalar	First Node on the Surface	FCOS		I
NP2	--	Scalar	Second Node on the Surface	FCOS		I
NP3	--	Scalar	Third Node on the Surface	FCOS		I
NPBB(I)	--	Array	Global Node Number on the I-th Boundary Node	GM3D DATAIN SURF SFLOW NDTAU ADVTRN ADVBC		M M O I I I I
NPCB(NP)	--	Array	Global Nodal Number of the NP-Cauchy Node on Input. Then it is Changed to Contain the Boundary Node Number	GM3D DATAIN SFLOW ADVBC		M M I I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NPDB(NP)	--	Array	Global Node Number of the NP-Dirichlet Node on Input. Then it is Changed to Contain the Boundary Node Number	GM3D DATAIN BC ADVBC SFLOW		M M I I I
NPITER	--	Scalar	Number of Blockwise Iterations Allowed		CINTE	
NPNB(NP)	--	Array	Global Nodal Number of the NP-Neumann Node on Input. Then it is Changed to Contain the Boundary Node Number.	GM3D DATAIN SFLOW		M M I
NPR	--	Scalar	Number of Profiles	ALLFCT		I
NPROB	--	Scalar	Problem Number	STORE		I
NPVB(NP)	--	Array	Global Nodal Number of the NP-Variable Node on Input. Then it is Changed to Contain the Boundary Node Number	GM3D DATAIN SFLOW ADVBC		M M I I
NPW(I)	--	Array	Global Node Number of the I-th Well Node	GM3D DATAIN ASEMBL SFLOW		M M I I
NRDP	--	Scalar	Number of Data Points on Rainfall Profiles		CVBC	
NREGN	--	Scalar	Number of Subregions		LGEOM	
NRPR	--	Scalar	Number of Rainfall Profiles		CVBC	
NSDP	--	Scalar	Number of Data Points in Any Element Source/ Sink Profile		CELS	
NSEL	--	Scalar	Number of Source/Sink Elemente		CELS	
NSPR	--	Scalar	Number of Source/Sink Profiles		CELS	
NTAU	--	Scalar	Number of Subtime Steps	NDTAU ADVTRN		O I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NTI	--	Scalar	Number of Time Increments		CGEOM	
NTNPLR(K)	--	Array	Total Number of Nodes for the K-th Subregion Including Interior, Global Boundary, and Intraboundary Nodes	GM3D DATAIN PAGEN		M M O
NTYPE	--	Scalar	Number of Integers to be Read	READN		
NVES	--	Scalar	Number of Variable Boundary Element Sides	CVBC		
NVNP	--	Scalar	Number of Variable Boundary Nodal Points	CVBC		
NWDP	--	Scalar	Number of Data Points in Any Point-Source Profile		CNPS	
NWNP	--	Scalar	Number of Wells		CNPS	
NWPR	--	Scalar	Number of Well Source Profiles		CNPS	
OME	--	Scalar	Iteration Parameter for a Non-Linear Equation	BLKITR	CREAL	I
OMI	--	Scalar	Relaxation Parameter for Pointwise Solution		CREAL	
PR(MXPR)	L/T,L, **M/L^3**	Array	Profile Value at Time t	ALLFCT		O
PRF(MXDP, MXPER)	L/T,L, M/L^s	Array	Profile Value of the Data Point on the Profile	ALLFCT		I
PROP(1,I)	**L^3/M**	Array	Distribution Coefficient or Freudlich K or Langmuir K	GM3D DATAIN AFABTA FLUX ASEMBL SFLOW THNODE		M M I I I I I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
PROP(2,I	M/L^3	Array	Bulk Density	GM3D		M
				DATAIN		M
				AFABTA		I
				FLUX		I
				ASEMBL		I
				SFLOW		I
THNODE		I				
PROP(3,I)	L	Array	Longitudinal Dispersivity	GM3D		M
				DATAIN		M
				AFABTA		I
				FLUX		I
				ASEMBL		I
				SFLOW		I
				THNODE		I
PROP(4,I)	L	Array	Transverse Dispersivity	GM3D		M
				DATAIN		M
				AFABTA		I
				FLUX		I
				ASEMBL		I
				SFLOW		I
				THNODE		I
PROP(5,I)	L^2/T	Array	Molecular Diffusion Coefficient	GM3D		M
				DATAIN		M
				AFABTA		I
				FLUX		I
				ASEMBL		I
				SFLOW		I
				THNODE		I
PROP(6,I)	--	Array	Tortuosity	GM3D		M
				DATAIN		M
				AFABTA		I
				FLUX		I
				ASEMBL		I
				SFLOW		I
				THNODE		I
PROP(7,I)	1/L	Array	Decay Constant	GM3D		M
				DATAIN		M
				AFABTA		I
				FLUX		I
				ASEMBL		I
				SFLOW		I
				THNODE		I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Unite	Type	cri	Sub-routine	Common Block	I,M,O
PROP(8,I)	--	Array	Freundlich N or Langmuir SMAX	GM3D DATAIN AFABTA FLUX ASEMBL SFLOW THNODE		M M I I I I I
QA(8,8)	--	Array	An Element Matrix	Q8		O
Q,AA(8,8)	--	Array	An Element Matrix	Q8		O
QB(8,8)	--	Array	An Element Matrix	Q8DV Q8		O O
QBMP	M/L²/T	Scalar	Flux or Concentration of the Boundary Side	Q4CNVB Q4ADB		I I
QC(8,8)	--	Array	An Element Matrix	Q8		O
QCB(I)	M/L²/T	Array	Value of Cauchy Flux at the Present Time of the I-th Cauchy Flux Profile	GM3D BC ADVBC		M I I
QCBF(I,J)	M/T/L²	Array	Flux of the I-th Data Point in the J-th Cauchy Flux vs. Time Profile	GM3D DATAIN		M M
QDM	--	Scalar	Integration of Local Variable S	Q8R		O
QNB(I)	M/L²/T	Array	Value of Neumann Flux at the Present Time of the I-th Neumann Flux Profile	GM3D BC		M I
QNBF(I,J)	M/T/L²	Array	Flux of the I-th Data Point in the J-th Neumam Flux vs. Time Profile	GM3D DATAIN		M M
QR(8)	--	Array	An Element Load Vector	Q8		O
QRM	--	Scalar	Integration of TH*C	Q8R		O
QRX(8)	--	Array	Element Lead Vector for x-Flux	Q8DV		O
QRY(8)	--	Array	Element Load Vector for Y-Flux	Q8DV		O
QRZ(8)	--	Array	Element Load Vector for z-Flux	Q8DV		O

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
QV(8,8)	--	Array	An Element Matrix	Q8		O
R(MAXNP)	--	Array	Load Vector	SOLVE		M
RHOB	M/L^3	Scalar	Bulk Density of the Material in Element	Q8		I
RI(N)	--	Array	Working Array Used in Subroutines BLKITR and ADVBC	GM3D BLKITR ADVBC		M O M
RL(N)	--	Array	Working Array Used in Subroutine ADVBC	GM3D ADVBC		M M
RLD(N)	--	Array	An Array to Store the Right Hand Side of the N-th Equation of the Assembled Global Load Vector	GM3D ASEMBL BC		M O O
RLDG MAXNP)	--	Array	Global Load Vector	BLKITR		I
RLDL(N)	--	Array	Assembled Load Vector for a Subregion	GM3D BLKITR		M I
RQ(4)	M/T	Array	Integrated Flux at Four Nodes of the Element Surface	Q4CNVB Q4BB		O O
RQI(4)	$M/L^2/T$	Array	Material-Flux at Four Nodes of the Surface	Q4ADB		O
RQL(4)	$L^3/L^2/T$	Array	Flow-Flux at Four Nodes of the Surface	Q4ADB		O
S0S(I,1)	$L^3/L^2/T$	Array	Source Flow Rate of the I-th Profile at Time t	GM3D ASEMBL SFLOW		M I I
S0S(I,2)	L'/L'/'I'	Array	Source Concentration of the I-th Profile at Time t	GM3D ASEMBL SFLOW		M I I
SOSC	M/L^3	Scalar	Source Concentration	Q8		I
SOSCP	M/L^3	Scalar	Concentration in Element-Source	Q8R		I
SOSF (I,J,l)	L'/TIL'	Array	Source Flow Rate of the I-th Data Point in the J-th Profile	GM3D DATAIN		M M

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
SOSF (I,J,2)	M/L'	Array	Source Concentration of the I-th Data Point in the J-th Profile	GM3D DATAIN		M M
SOSM	M/T	Scalar	Integration of Q*Cin	Q8R		O
SOSQ	L^3/T	Scalar	Element-Source Flow Rate	Q8		I
SOSQP	L^3/T	Scalar	Element-Source Flow Rate	Q8R		I
SS	--	Scalar	XSI-Coordinate of the Gaussian Point	SHAPE		I
SWQ(8)	M/T	Array	Iterate of the Adsorbed Concentration at Eight Gaussian Points of the Element	Q8		I
T	T	Scalar	Time	ALLFCT		I
TAU	--	Scalar	Tortuosity	Q8		I
TCDBF(I,J)	T	Array	Time of the I-th Data Point in the J-th Dirichlet Concentration vs. Time Profile	GM3D DATAIN		M M
TCVBF(I,J)	T	Array	Time of the I-th Data Point in the J-th Variable Concentration vs. Time Profile	GM3D DATAIN		M M
TDTCH(I)	T	Array	Time of the I-th Time to Reset Time-Step Size (= DELTO)	GM3D DATAIN		M M
TFLOW	M/L	Scalar	Total Flow		CFLOW	
TH(I,M)	--	Array	Moisture Content at the I-th Node of the M-th Element	GM3D FLUX ASEMBL SFLOW THNODE		M I I I I
THG(8)	--	Array	Moisture Content at Eight Gaussian Points of the Element	Q8 Q8R		I I
THN(N)	--	Array	Moisture Content at the N-th Node	GM3D THNODE NDTAU		M O I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
				ADVTRN		I
				ADVBC		I
THP(I,M)	--	Array	Value of TH(I,M) at the Previous Time	GM3D		M
				ASEMBL		I
				THNODE		I
THQ(8)	--	Array	Moisture Content at Eight Points of the Element	Q8DV		I
TIME	T	Scalar	Time	DATAIN		M
				PRINTT		I
				STORE		I
TITLE	--		Title of the Problem	STORE		I
TMAX	T	Scalar	Maximum Value of Time		CREAL	
TOLA	L	Scalar	Steady-State Tolerance		CREAL	
TOLB	L	Scalar	Transient-State Tolerance	BLKITR	CREAL	I
TPRF(MXDP, MXPR)	T	Array	Time of the Data Point on the Profile	ALLFCT		I
TQCBF(I,J)	T	bray	Time of the I-th Data Point in the J-th Cauchy Flux vs. Time Profile	GM3D		M
				DATAIN		M
TQNBF(I,J)	T	Array	Time of the I-th Data Point in the J-th Neumam Flux vs. Time Profile	GM3D		M
				DATAIN		M
TSOSF(I,J)	T	Array	Time of the I-th Data Point in the J-th Element Source Profile	GM3D		M
				DATAIN		M
TT	--	Scalar	Eta-Coordinate of the Gaussian Point	SHAPE		I
TWSSF(I,J)	T	Array	Time of the I-th Data Point in J-th Well Source Profile	GM3D		M
				DATAIN		M
UU	--	Scalar	Zeta-Coordinate of the Gaussian Point	SHAPE		I
VX(N)	UT	Array	X-Component Velocity at the N-th Node	GM3D		M
				FLUX		I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
				AFABTA		I
				ASEMBL		I
				BC		I
				NDTAU		I
				ADVTRN		I
				ADVBC		I
VXP(N)	L/T	Array	Value of VX(N) at the Previous Time	GM3D		M
				AFABTA		I
				ASEMBL		I
				BC		I
				NDTAU		I
				ADVTRN		I
				ADVBC		I
VXQ(8)	L/T	Array	X-Velocity of Eight Nodes of the Element	Q8DV		I
				Q8		I
				Q4CNVB		I
				Q4ADB		I
VY(N)	L/T	Array	Y-Component Velocity at the N-th Node	GM3D		M
				AFABTA		I
				FLUX		I
				ASEMBL		I
				BC		I
				NDTAU		I
				ADVTRN		I
				ADVBC		I
VYP(N)	L/T	Array	Value of VY(N) at the Previous Time	GM3D		M
				AFABTA		I
				ASEMBL		I
				BC		I
				NDTAU		I
				ADVTRN		I
				ADVBC		I
VYQ(8)	L/T	Array	Y-Velocity of Eight Nodes of the Element	Q8DV		I
				Q8		I
				Q4CNVB		I
				Q4ADB		I
VZ(N)	L/T	Array	Z-Component Velocity at the N-th Node	GM3D		M
				AFABTA		I
				FLUX		I
				ASEMBL		I
				BC		I
				NDTAU		I
				ADVTRN		I
				ADVBC		I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	LMQ
VZP(N)	L/T	Array	Value of VZ(N) at the Previous Time	GM3D AFABTA ASEMBL BC NDTAU ADVTRN ADVBC		M I I I I I I
VZQ(8)	L/T	Array	Z-Velocity of Eight Nodes of the Element	Q8DV Q8 Q4CNVB Q4ADB		I I I I
W(8)	--	Array	Weighting Function at Eight Points of the Element	SHAPE		O
WETAB(J, M)	--	Array	Weighting Factor for the J-th Side of the M-th Element	GM3D AFABTA FLUX ASEMBL		M O I I
WSS(I,l)	L^3/T	Array	Well Source Flow Rate of the I-th Profile at Time t	GM3D ASEMBL SFLOW		M I I
WSS(I,2)	M/L^3	Array	Well Source Concentration at the I-th Profile	GM3D ASEMBL SFLOW		M I I
WSSF (J,I,l)	L^3/T	Array	Well Source Flow Rate of the I-th Data Point in the J-th Profile	GM3D DATAIN		M M
WSSF (J,I,2)	M/L^3	Array	Well Source Concentration of the I-th Data Point in the J-th Profile	GM3D DATAIN		M M
WWRK(N)	--	Array	Working Array Used in Subroutine THNODE	GM3D THNODE		M O
X(N)	L	Array	X-Coordinate of the N-th Node	GM3D DATAIN SURF AFABTA FLUX ASEMBL BC SFLOW STORE THNODE		M M I I I I I I I I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
				NDTAU		I
				ADVTRN		I
				MPLOC		I
				XS13D		I
				ADVBC		I
XP	L	Scalar	X-Coordinate of the Fictitious Particle	MPLOC		I
				FCOS		I
				XSI3D		I
XQ(8)	L	Array	X-Coordinate at Eight Points of the Element	Q8DV		I
				Q8		O
				SHAPE		I
				Q4CNVB		I
				Q4BB		I
				Q8R		I
				Q4ADB		I
XSI	--	Scalar	Local Coordinate of the Particle	XSI3D		O
Y(N)	L	Array	Y-Coordinate of the N-th Node	GM3D		M
				DATAIN		M
				SURF		I
				AFABTA		I
				FLUX		I
				ASEMBL		I
				BC		I
				SFLOW		I
				STORE		I
				THNODE		I
				NDTAU		I
				ADVTRN		I
				MPLOC		I
				FCOS		I
				XSI3D		I
				ADVBC		I
YP	L	Scalar	Y-Coordinate of the Fictitious	MPLOC		I
				FCOS		I
				XSI3D		I
YQ(8)	L	Array	Y-Coordinate at Eight Points of the Element	Q8DV		I
				Q8		O
				SHAPE		I
				Q4CNVB		I
				Q4BB		I
				Q8R		I
				Q4ADB		I

TABLE D-2. 3DLEWASTE PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Unite	Type	Description	Sub-routine	Common Block	I,M,O
Z(N)	L	Array	Z-Coordinate of the N-th Node	GM3D		M
				DATAIN		M
				SURF		I
				AFABTA		I
				FLUX		I
				ASSEMBL		I
				BC		I
				SFLOW		I
				STORE		I
				THNODE		I
				NDTAU		I
				ADVTRN		I
				MPLOC		I
				FCOS		I
				XSI3D		I
				ADVBC		I
ZP	L	Scalar	Z-Coordinate of the Fictitious Particle	MPLOC		I
				FCOS		I
				XSI3D		I
ZQ(8)	L	Array	Z-Coordinate at Eight Points of the Element	Q8DV		I
				Q8		O
				SHAPE		I
				Q4CNVB		I
				Q4BB		I
				Q8R		I
				Q4ADB		I
ZTA	--	Scalar	Local Coordinate of the Particle	XSI3D		O

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