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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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FOREWORD

As environmental controls become more costly to implement and the penalties of judgement 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 which 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, is needed.

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 (A Three-dimensional Finite Element Model of WATER Flow through Saturated-Unsaturated Media) simulates subsurface flows, whereas 3DLEWASTE (A Hybrid Three-Dimensional Lagrangian-Eulerian Finite Element Model of WASTE Transport through Saturated-Unsaturated Media) models contaminant transport. Both codes 1) treat heterogeneous and anisotropic media consisting of as many geologic formations as desired, 2) consider both distributed and point sources/sinks that are spatially and temporally dependent, and 3) 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 on 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, 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. The 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 Scarbrough 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 DELINEATION

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 judgement or an established distance criterion.
- **Calculated fixed radius**, in which the radius of a circle around the well is determined from an equation which 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 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 which 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 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 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 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 modeled using 3DFEMWATER/3DLEWASTE.

1.2 THE 3DFEMWATER/3DLEWASTE WHPA MODEL

3DFEMWATER (A 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 fixed-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 on 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 (A 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 upwind 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, while 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 spatially and temporally distributed, 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, 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 3DFMEWATER/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 inferred 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 conductivities.

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 types. 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 finely 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 INSTALFW (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 EX PRESS (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 CEAM, 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 = 1,048,576 bytes
1 b = 1 byte

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
  Center for Exposure Assessment Modeling

U.S. Environmental Protection Agency
960 College Station Road
Environmental Research Laboratory
Athens, GA 30605-2720

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:

- 300/1200/2400/9600/14400 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 10mb free hard disk storage.

2.4.2 Run Time Requirements

- 486 compatible microcomputer.
- MS or PC DOS version 3.30 or higher.
- 640k base memory.
- 25 mb combination of extended memory and/or disk storage space
- math coprocessor

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 706/546-3210 for assistance.
- Use of the CEAM electronic bulletin board system (BBS), contact the BBS system

operator (SYSOP) at 706/546-3590.

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

- Other support available through CEAM, contact Mr. Dermont Bouchard, CEAM Manager:

  - By mail at the following address:

    Center for Exposure Assessment Modeling (CEAM)
    Environmental Research Laboratory
    U.S. Environmental Protection Agency
    960 College Station Road
    Athens, Georgia 30605-2720

  - By telephone at 706/546-3130.

  - By fax at 706/546-3340.

  - 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).

A user will be on their own if he/she attempts 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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- Sun and SunOS are registered trademarks of Sun Microsystems, Inc.
- SPARC is a registered trademark of SPARC International, Inc.
- UNIX is a registered trademark of American Telephone and Telegraph.
- SVS FORTRAN-77 is a trademark of Silicon Valley Software.
- PRIME and PRIMOS are trademarks of Prime Computers, Inc.
- Microsoft, RAMDRIVE, HIMEM, MS, and MS-DOS are registered trademarks of Microsoft Corporation.
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- RM/FORTRAN is a trademark of Language Processors, Inc.
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- 386 and 486 are trademarks of Intel Corporation.
- U.S. Robotics is a registered trademark and Courier HST is a trademark of U.S. Robotics, Inc.

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:

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

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: