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Standard Guide for Documenting a Ground-Water Modeling Code[1]

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ε[1] NOTE—Paragraph 1.6 was added editorially in October 1998.

1. Scope

1.1 This guide covers suggested components of the documentation of a ground-water modeling code. Documentation of a ground-water modeling code consists of textual and graphical information recorded during its design, development, and maintenance regarding its capabilities, development history, theoretical foundation, operation, and verification. It is the principal instrument for those involved in its development and use, such as code development and maintenance staff, network managers, code users and project managers, to communicate regarding all aspects of the software.

1.2 This guide presents the major steps in preparing the documentation of a ground-water modeling code. It discusses the various documentation audiences and addresses the role of printed documentation versus documentation in electronic form.

1.3 This guide is one of a series of guides on ground-water modeling codes and their applications, such as D 5447, D 5490, D 5609, D 5610, D 5611, and D 5718.

1.4 This guide is not intended to be all inclusive. If offers a series of options and considerations, but does not specify a course of action. Documenting certain codes may require supplemental information or replacement of documentation sections by more appropriate elements. This guide should not be used as a sole criterion or basis of comparison, and does not replace or relieve professional judgement in preparing or evaluating documentation of ground-water modeling software.

1.5 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to its use.*

1.6 *This guide offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience and should be used in conjunction with professional judgment. Not all aspects of this guide may be applicable in all circumstances. This ASTM standard is not intended to represent or replace the standard of care by which the adequacy of a given professional service must be judged, nor should this document be applied without consideration of a project's many unique aspects. The word "Standard" in the title of this document means only that the document has been approved through the ASTM consensus process.*

2. Referenced Documents

2.1 *ASTM Standards:*

D 653 Terminology Relating to Soil, Rock, and Contained Fluids[2]

D 5447 Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem[2]

D 5490 Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information[2]

D 5609 Guide for Defining Boundary Conditions in Ground-Water Flow Modeling[2]

D 5610 Guide for Defining Initial Conditions in Ground-Water Flow Modeling[2]

D 5611 Guide for Performing a Sensitivity Analysis for a Ground-Water Flow Model Application[2]

D 5718 Guide for Documenting a Ground-Water Flow Model Application[3]

3. Terminology

3.1 *Definitions of Terms Specific to This Standard:*

3.1.1 *computer code (computer program)*—the assembly of numerical techniques, bookkeeping, and control language that represents the model from acceptance of input data and instructions to delivery of output.

3.1.2 *functionality*—of a ground-water modeling code, the set of functions and features the code offers the user in terms of model framework geometry, simulated processes, boundary conditions, and analytical and operational capabilities.

3.1.3 *ground-water modeling code*—the non-parameterized computer code used in ground-water modeling to represent a non-unique, simplified mathematical description of the physical framework, geometry, active processes, and boundary conditions present in a reference subsurface hydrologic system.

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[2] *Annual Book of ASTM Standards*, Vol 04.08.

[3] *Annual Book of ASTM Standards*, Vol 04.09.

3.2 For definitions of other terms used in this guide, see Terminology D 653.

4. Significance and Use

4.1 Ground-water modeling has become an important methodology in support of the planning and decision-making processes involved in ground-water management. Ground-water models provide an analytical framework for obtaining an understanding of the mechanisms and controls of ground-water systems and the processes that influence their quality, especially those caused by human intervention in such systems. Increasingly, models are an integral part of water resources assessment, protection and restoration studies and provide essential and cost-effective support for planning and screening of alternative policies, regulations, and engineering designs affecting ground-water **(1).**[4]

4.2 Successful ground-water management requires that decisions be based on the use of technically and scientifically sound methods for data collection, information processing, and interpretation, and that these methods are properly integrated. As computer codes are essential building blocks of modeling-based management, it is crucial that before such codes are used as planning and decision-making tools, their performance characteristics are established and their theoretical foundation, capabilities and use documented.

4.3 Good code documentation ensures scientific rigor and implementational quality in the development of a code **(2)**. Complete and well-written documentation shortens the learning curve for new users, provides answers to questions from project managers, and supports efficient code selection. Well-structured and indexed documentation provides rapid answers for initiated users. This standard guide is intended to encourage comprehensive and consistent documentation of a ground-water modeling code.

4.4 Earlier surveys of computer models and assessment of specific models indicate that the documents that are supposed to describe and explain these models and their use are lacking in detail, inconsistent in their contents, incomplete with respect to user instructions, inefficient with respect to indexing and structure, and often difficult to obtain **(3)**. This still applies to the documentation of many of the ground-water modeling programs recently released, or frequently used **(4)**.

5. Code Development Process in Ground-Water Modeling

5.1 In ground-water modeling, code development consists of the following: definition of design criteria and determining applicable software standards and practices; the development of algorithms and program structure; computer programming; preparation of documentation; code testing; and independent review of scientific principles, mathematical framework, software, and documentation **(1,4)**.

5.2 The development of a specific ground-water modeling code may be part of a research or development project, based on an existing mathematical model, or derived from an existing set of modeling codes.

5.3 Code testing is an integral part of code development. During the programming phase testing is focussed on individual algorithms, subroutines, functions and other program elements. At the end of the initial programming phase, the code is extensively tested.

5.4 The preparation of the program documentation starts at the beginning of the code development process and is integral to all stages of code development. Specifically, documentation of theoretical foundation, code design, capabilities and program structure are best prepared and evaluated during the design and programming phases of the project. Documentation regarding the operation and performance of the code are best prepared before and during initial testing by code developers.

5.5 The final step in code development is independent review and testing.

6. Code Documentation Requirements

6.1 Following are the main purposes of software documentation **(3)**: to record technical information that enables system and program changes to be made quickly and effectively; to assist the (potential) users in understanding what the program is about and what it can do, so that they can determine whether it serves their needs; to enable code users to effectively apply the program to their project(s); to facilitate auditing and verification of program operations, that is, code evaluation; to enable programmers and system analysts, other than software originators, to work on the programs; to provide software development managers with information to review at significant developmental milestones so that they may determine that project requirements have been met and that resources should continue to be expended; to reduce the disruptive effects of personnel turnover during development and use of the software; and to facilitate understanding among developers, users and project managers by providing information about maintenance (that is, required software modifications), training, and operation of the software.

6.2 Documentation of a ground-water modeling code may be comprised of several elements such as internal or published reports, published articles, textbooks, electronic texts, and software help systems. If a program's documentation consists of more than one such element, it is recommended to include a section referencing all elements that constitutes the code's documentation.

6.3 Documentation of a ground-water modeling code should be informative, well-structured (that is, specific topics are easy to find), and well-written (that is, topics are easy to understand).

6.4 Documentation of a gound-water modeling code should include sections on the following **(5)**: development purpose; theoretical framework; mathematical/logic methods and computer algorithms employed; model construction and site-specific data required to control the code; analysis of the sensitivity of computed variables for variations in model parameters; verification conducted and operational evaluations performed; example applications and demonstration test cases; installation, input preparation and code execution instructions; and methods to review input data and results. A summary of

[4] The boldface number given in parentheses refer to a list of references at the end of the text.

code capabilities (that is, an overview of the code's functionality), a description of the development history, a trouble-shooting guide, and a detailed index are also useful elements of code documentation.

6.5 Comprehensive software documentation typically consists of four types of manuals providing information aimed at project managers, software users, (problem) analysts, and programmers, respectively **(6)**. In ground-water modeling, such information is often included in a single document, containing specific sections for the different audiences; frequently, the program user is the same as the problem analyst (that is, the hydrogeologist).

6.5.1 Project managers find important information in a summary section containing a general description, a discussion of code development history, a testing report, and a discussion of current and future applications.

6.5.2 The user's instructions section, sometimes published as a separate user's manual, contains a comprehensive description of code functions and capabilities, code input data requirements and format, types of output and output controls, code execution details, sample runs, and a trouble-shooting guide, and code verification and performance evaluation information.

6.5.3 An effective user's manual enables the (non-programmer) user to perform the following **(2, 3)**: thoroughly understand the inner workings of the code; accurately formulate a problem in terms of code input required; prepare the data for code input (data requirements, data preparation, description of input formats, array dimensions and problem size limitations); run the code to obtain desired output (for example, discussion of execution and output control parameters, selection of data units and corresponding file requirements, listing of computer requirements and installation instructions, discussion of numerical precision of the code and accuracy of results), and provide information for interpretation of output. Such a user's manual includes a complete set of operating instructions, as well as instructions with respect to model construction.

6.5.3.1 *General Description*—A comprehensive description of what the model is supposed to do (typically called "code functions and capabilities" or "code functionality"), why it has been developed, what its intended use is, and the general magnitude of its applicability in terms of major assumptions and limitations. This section is also the appropriate place to describe the relationship to other software required for its preparation, operation, or output analysis.

6.5.3.2 *Theoretical Foundation/Methodology*—A detailed description of how the model accomplishes its intended purpose. These details are preferably provided in the sequence in which they are performed in the code. It includes the theoretical model and the underlying assumptions, as well as the mathematical representation (that is, the mathematical model). The mathematical description should include the simplifications made to the theoretical model, the mathematical expressions (that is, governing equations, boundary conditions, and solution methods), the logic of the model, and the computer algorithms. In many instances, it will be useful to include a flow chart of the general workings of the program.

6.5.3.3 *Model Construction*—A description of ground-water model construction requirements and considerations, that is, considerations in translating a user problem into a code's input format (for example, grid design and accuracy, boundary and initial conditions, time step selection and and accuracy, and application limitations).

6.5.3.4 *Specific Data Requirements*—A description of the type of information required by the program, including a description of spatial and temporal distribution, the overall data structure, the data media, general data limitations, and specific input parameters (that is, their meaning, typical range, and use in the code, including restrictions or bounds on the values). It should address issues related to unit conversion and format conversion, if applicable.

6.5.3.5 *Output Description*—A general description of the output structure, types of (optional) output, and names and characteristics of output files.

6.5.3.6 *Control Parameters*—A description of all code operation control parameters, including solution parameters, output option selection parameters, and other user-selectable code function switches.

6.5.3.7 *Input Formats*—Many programs require a specific order in which the input needs to be prepared. In addition, some codes require the input data to follow a predetermined format. The user's manual should include a description of all input formats, if this information is required to prepare the input files for the program.

6.5.3.8 *Verification and Performance Evaluation*—A discussion on the performed verification (that is, type of tests, completeness of testing, test problem descriptions, and evaluation of test results) **(7)**.

6.5.3.9 *Example Simulations*—The presence of detailed discussions of example or verification problems in the user's manual is a major benefit to the unacquainted user. Such discussions should cover model construction, selection of input parameters, the input data as they appear in the input file(s), and a hard-copy of relevant parts of the output file(s).

6.5.3.10 A practical user's manual includes a section containing run-time error message an explanation of possible causes, and instruction how to correct them.

6.5.3.11 *Table of Contents/Index*—A detailed table of contents and a comprehensive index improves the use of a user's manual.

6.5.4 The programmer's instructions should contain code specifications, a code description in terms of objectives and structure, program flow, a description of coded routines and algorithms, a description of data flow and data handling, source listing, and error messages. This includes information on the following: computer language, operating system/development platform, compiler/linker version; files names, file structure, format/type, contents and operational purpose; flow charts representing code logic, file usage; parameter/variable lists (names, type-integer, etc-, meaning, units); initialization and code array dimensioning procedures; routines and functions (brief description, size, entries, common arrays and variables); use of libraries, if present; and a description of potential problems, including for porting to other systems. The code

itself should be efficiently structured and internally well-documented; where possible, self-explanatory parameter, variable, subroutine and function names should be used.

7. Keywords

7.1 computer code; documentation; ground-water modeling

REFERENCES

(**1**) National Research Council (NRC), Committee on Ground Water Modeling Assessment, Water Science and Technology Board, *Ground Water Models: Scientific and Regulatory Applications*, National Academy Press, Washington, DC, 1990

(**2**) Simmons, C.R., and Cole, C.R., *Guidelines for Selecting Codes for Ground-Water Transport Modeling of Low-Level Waste Burial Sites; Volume 1– Guideline Approach*, PNL-4980 Vol. 1. Pacific Northwest Laboratory, Richland, Washington, 1985.

(**3**) Gass, S.I., "Computer Model Documentation: A Review and an Approach," *NBS Special Publ. 500–39*, Inst. for Computer Science and Technology, Nat. Bur. of Standards, U.S. Dept of Commerce, Washington, DC, 1979.

(**4**) van der Heijde, P.K.M., and Elnawawy, O.A., "Quality Assurance and Quality Control in the Development and Application of Ground-Water Models, *EPA/600/R-93/011*, R.S. Kerr Environmental Research Laboratory, U.S. Environmental Protection Agency, Ada, OK, 1992.

(**5**) Siling, S.A., "Final Technical Position on Documentation of Computer Codes for High-level Waste Management," *NUREG/CR-0856–F*, Off. of Nuclear Material Safety and Safeguards, U.S. Nuclear Regulatory Commission, Washington, DC, 1983.

(**6**) Federal Computer Performance Evaluation and Simulation Center (FEDSIM), "Computer Model Documentation Guide," *NBS Special Publ. 500–73*, Inst. for Computer Science and Technology, Nat. Bureau of Standards, U.S. Dept. of Commerce, Washington, DC, 1983.

(**7**) van der Heijde, P.K.M., and Kanzer, D.A., *Ground-Water Model Testing: Systematic Evaluation and Testing of Code Functionalityand Performance. EPA/600/R-97/007*, R.S. Kerr Environmental Research Laboratory, U.S. Environmental Protection Agency, Ada, OK, 1997.