



Standard Guide for Describing the Functionality of a Ground-Water Modeling Code¹

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^{ε1} NOTE—Paragraph 1.7 was added editorially in October 1998.

1. Scope

1.1 This guide presents a systematic approach to the classification and description of computer codes used in ground-water modeling. Due to the complex nature of fluid flow and biotic and chemical transport in the subsurface, many different types of ground-water modeling codes exist, each having specific capabilities and limitations. Determining the most appropriate code for a particular application requires a thorough analysis of the problem at hand and the required and available resources, as well as a detailed description of the functionality of potentially applicable codes.

1.2 Typically, ground-water modeling codes are nonparameterized mathematical descriptions of the causal relationships among selected components of the aqueous subsurface and the chemical and biological processes taking place in these systems. Many of these codes focus on the presence and movement of water, dissolved chemical species and biota, either under fully or partially saturated conditions, or a combination of these conditions. Other codes handle the joint movement of water and other fluids, either as a gas or a nonaqueous phase liquid, or both, and the complex phase transfers that might take place between them. Some codes handle interactions between the aqueous subsurface (for example, a ground-water system) and other components of the hydrologic system or with nonaqueous components of the environment.

1.3 The classification protocol is based on an analysis of the major function groups present in ground-water modeling codes. Additional code functions and features may be identified in determining the functionality of a code. A complete description of a code's functionality contains the details necessary to understand the capabilities and potential use of a ground-water modeling code. Tables are provided with explanations and examples of functions and function groups for selected types of codes. Consistent use of the descriptions provided in the classification protocol and elaborate functionality analysis form the basis for efficient code selection.

1.4 Although ground-water modeling codes exist for simulation of many different ground-water systems, one may

encounter situations in which no existing code is applicable. In those cases, the systematic description of modeling needs may be based on the methodology presented in this guide.

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

1.6 Complete adherence to this guide may not be feasible. For example, research developments may result in new types of codes not yet described in this guide. In any case, code documentation should contain a section containing a complete description of a code's functions, features, and capabilities.

1.7 *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 Fluids²
- D 5447 Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem³
- D 5490 Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information³
- D 5609 Guide for Defining Boundary Conditions in Ground-Water Flow Modeling³
- D 5610 Guide for Defining Initial Conditions in Ground-Water Flow Modeling³
- D 5611 Guide for Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application³
- D 5718 Guide for Documenting a Ground-Water Flow Model Application³

¹ This guide is under the jurisdiction of ASTM Committee D-18 on Soil and Rock and is the direct responsibility of Subcommittee D18.21 on Ground Water and Vadose Zone Investigations.

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² Annual Book of ASTM Standards, Vol 04.08.

³ Annual Book of ASTM Standards, Vol 04.09.

3. Terminology

3.1 *Definitions*—For definitions of terms used in this guide, see Terminology D 653.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *analytical model, n*—a model that uses closed form solutions to the governing equations applicable to ground-water flow and transport processes.

3.2.2 *backtracking model, n*—an application of a mathematical model for determining ground-water system stresses and boundary conditions when the system parameters are known and the system responses are either known or bounded.

3.2.3 *finite difference model, n*—a type of approximate, numerical model that uses a discrete technique for solving the governing partial differential equation (PDE) consisting of replacing the continuous domain of interest by a finite number of regular-spaced mesh or grid points (that is, nodes) representing volume-averaged subdomain properties, approximating the derivatives of the PDE for each of these points using finite differences, and solving the resulting set of linear or nonlinear algebraic equations using direct or iterative matrix solving techniques.

3.2.4 *finite element model, n*—a type of approximate, numerical model that uses a discrete technique for solving the governing partial differential equation (PDE) wherein the domain of interest is represented by a finite number of mesh or grid points (that is, nodes), and information between these points is obtained by interpolation using piecewise continuous polynomials. The resulting set of linear or nonlinear algebraic equations is solved using direct or iterative matrix solving techniques.

3.2.5 *functionality, n*—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.

3.2.6 *ground-water flow model, n*—an application of a mathematical model to represent a regional or site-specific ground-water flow system.

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

3.2.8 *heat transport model, n*—an application of a mathematical model to represent the movement of heat or energy in a ground-water system.

3.2.9 *inverse model, n*—an application of a mathematical model designed for evaluating ground-water system parameters and stresses by minimizing the differences between computed and observed system responses.

3.2.9.1 *Discussion*—The term *inverse model* refers in general to a numerical code that incorporates a systematic, automated procedure to minimize the differences between observed and computed system responses. This type of model also is known as a parameter estimation model or parameter identification model. Typically, these models are based on numerical simulation of the ground-water system. Aquifer test and tracer test analysis software are often based on analytical

models of the ground-water system. Since they include automated procedures to estimate the system parameters, they can be considered *inverse* models.

3.2.10 *numerical model, n*—a model that uses numerical methods to solve the governing equations of the applicable problem.

3.2.11 *prediction model, n*—an application of a mathematical model designed for predicting ground-water system responses, assuming the system parameters are known. These models are based on a so-called forward or direct mathematical formulation of the physical processes.

3.2.12 *solute transport model, n*—an application of a mathematical model to represent the movement of chemical species dissolved in ground water.

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.⁴

4.2 There are many different ground-water modeling codes available, each with their own capabilities, operational characteristics, and limitations. If modeling is considered for a project, it is important to determine if a particular code is appropriate for that project, or if a code exists that can perform the simulations required in the project.

4.3 In practice, it is often difficult to determine the capabilities, operational characteristics, and limitations of a particular ground-water modeling code from the documentation, or even impossible without actual running the code for situations relevant to the project for which a code is to be selected due to incompleteness, poor organization, or incorrectness of a code's documentation.⁵

4.4 Systematic and comprehensive description of a code's features based on an informative classification provides the necessary basis for efficient selection of a ground-water modeling code for a particular project or for the determination that no such code exists. This guide is intended to encourage correctness, consistency, and completeness in the description of the functions, capabilities, and limitations of an existing ground-water modeling code through the formulation of a code

⁴ 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.

⁵ van der Heijde, P. K. M., and Kanzer, D. A., "Ground-water Model Testing: Systematic Evaluation and Testing of Code Functionality, Performance, and Applicability to Practical Problems," EPA/600/R-97/007, R.S. Kerr Environmental Research Laboratory, U.S. Environmental Protection Agency, Ada, Oklahoma, 1996.

classification system and the presentation of code description guidelines.

5. Classification of Ground-Water Modeling Codes

5.1 There are many ground-water modeling codes available designed to simulate, describe, or analyze different types of ground-water systems and problems. The descriptive information of such software can be divided in three groups.⁶

5.1.1 *General Software Information*, includes such items as code name, version number, and release date of current version; development team; supported computer platform(s) and requirements; software language(s) and requirements; availability conditions and distributors; and software support and maintenance;

5.1.2 *Simulation System Information*, refers to descriptions of the nature of the systems that can be simulated, the method of simulation, the computed variables, and the required model input; and,

5.1.3 *Performance Evaluation Information*, including the results of code verification, analysis of the sensitivity of the dependent variable for natural variations in system controls and system parameters (that is, system input), and listing of operational limitations.

5.2 To describe systematically the features of ground-water modeling codes, a classification is used based on simulation system information (see Table 1). Three primary categories of code features can be distinguished as follows:⁶

5.2.1 The (design) purpose(s) or objective(s) of the software;

5.2.2 The nature of the ground-water system that can be simulated with the software; and,

5.2.3 The mathematical framework.

5.3 *Objective-Oriented Classification*⁶ (see Table 1):

5.3.1 The purpose or objective of a ground-water modeling code can be defined in terms of the applicability of the code to certain types of ground-water management problems, the code's functional use, or its computational output.

5.3.2 Management objectives may include requirements, such as type of problems which may be simulated, type of calculations and level of resolution required, acceptable accuracy, representation of specific management strategies, and other technical, scientific, social, and economic objectives. In general, however, it is not practical to develop a standard classification and description system based on such management objectives, as these are taken more easily into account in the code selection process than in the code documentation phase.

5.3.3 By design, a code's functional-use objectives may be one or more of the following:

5.3.3.1 To enable evaluation of a new theory and related hypotheses as part of research;

5.3.3.2 To be used as a tool in education and demonstration of principles;

5.3.3.3 To be used as a generic tool for ground-water system characterization;

5.3.3.4 To be used as a generic tool for engineering design (for example, well fields, excavations, remedial actions, and so forth);

5.3.3.5 To be used as a site- or problem-dedicated tool (including site- or problem-specific data); and,

5.3.3.6 To be used as a generic or dedicated tool for policy or management strategy screening.

5.3.4 A classification based on computational output includes the following categories:

5.3.4.1 *Screening or Ranking Models*—Facilitating qualitative evaluation of relative merits and disadvantages of various management or engineering alternatives;

5.3.4.2 *Prediction Models*—Predicting system responses, assuming the system parameters (for example, hydraulic conductivity, storativity) and system stresses (for example, boundary conditions) are known (that is, independent field information); the most common variables computed by prediction models are hydraulic head, drawdown, pressure, velocity (vector), fluid flux (vector), stream- or pathlines, isochrones, contaminant fronts, contaminant concentration (in both liquid and solid phase), solute flux (vector), temperature, enthalpy, heat flux (vector), location of (saltwater/freshwater) interface, water balance, and chemical mass balance.

5.3.4.3 *Backtracking Models*—Determining system stresses and boundary conditions when the system parameters are known (from observation) and the system responses are either known or bounded, used to determine, among others, location and duration of a contaminant release, to reconstruct well-field pumping history, or to estimate aquifer recharge rates.

TABLE 1 Classification Categories for Ground-Water Modeling Software⁶

Code Design Objectives
Applicability of the software to certain types of ground-water management problems
Calculated variables:
Screening/ranking
Prediction
Backtracking
Inverse or parameter estimation
Optimization
Functional use:
Research
Education and demonstration
General system characterization
General engineering screening/design
Site/problem dedicated
Policy/strategy screening
Nature of Ground-Water System: Hydrogeological and Soil-Morphological Framework
Hydrostratigraphy:
Water-saturated versus partially saturated
Porous medium versus fractured rock
Single, simple system versus multilayered system of aquifers and aquitards or soils
(Leaky-) confined versus phreatic aquifer conditions
Heterogeneity, anisotropy
Boundaries and internal geometry
System boundaries: location and conditions (for example, recharge; ground-water divide; impermeable base; stream; pond; seepage face; springs; point, line, or patch contaminant or heat source; diffuse source, and so forth)

⁶ 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.