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## Standard Guide for Describing the Functionality of a Groundwater Modeling Code<sup>1</sup>

This standard is issued under the fixed designation D6033; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon ( $\epsilon$ ) indicates an editorial change since the last revision or reapproval.

### 1. ~~Scope~~ Scope\*

1.1 This guide presents a systematic approach to the classification and description of computer codes used in groundwater modeling. Due to the complex nature of fluid flow and biotic and chemical transport in the subsurface, many different types of groundwater 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, groundwater modeling codes are ~~nonparameterized~~ non-parameterized 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 groundwater 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 groundwater modeling codes. Additional code functions and features may be identified in determining the functionality of a code. A ~~complete~~ complete description of a ~~code's~~ code's functionality contains the details necessary to understand the capabilities and potential use of a groundwater 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 groundwater modeling codes exist for simulation of many different groundwater systems, one may encounter situations ~~in which no~~ where existing code is ~~available~~ or 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 groundwater modeling codes and their applications, such as Guides **D5447**, **D5490**, **D5609**, **D5610**, **D5611**, and **D5718**.

1.6 ~~Complete~~ Full 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, those cases,~~ code documentation should contain a section containing a ~~complete~~ full description of a ~~code's~~ 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.*

<sup>1</sup> This guide is under the jurisdiction of ASTM Committee **D18** on Soil and Rock and is the direct responsibility of Subcommittee **D18.21** on Groundwater and Vadose Zone Investigations.

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\*A Summary of Changes section appears at the end of this standard

## 2. Referenced Documents

### 2.1 ASTM Standards:<sup>2</sup>

- D653 Terminology Relating to Soil, Rock, and Contained Fluids
- D5447 Guide for Application of a Groundwater Flow Model to a Site-Specific Problem
- D5490 Guide for Comparing Groundwater Flow Model Simulations to Site-Specific Information
- D5609 Guide for Defining Boundary Conditions in Groundwater Flow Modeling
- D5610 Guide for Defining Initial Conditions in Groundwater Flow Modeling
- D5611 Guide for Conducting a Sensitivity Analysis for a Groundwater Flow Model Application
- D5718 Guide for Documenting a Groundwater Flow Model Application

## 3. Terminology

3.1 *Definitions*—For definitions of common terms used in this guide, see Terminology **D653**.

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 groundwater flow and transport processes.

3.2.2 *backtracking model, n*—an application of a mathematical model for determining groundwater 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 groundwater 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 *groundwater flow model, n*—an application of a mathematical model to represent a regional or site-specific groundwater flow system.

3.2.3 *groundwater modeling code, n*—the nonparameterized computer code used in groundwater 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.

<sup>2</sup> For referenced ASTM standards, visit the ASTM website, [www.astm.org](http://www.astm.org), or contact ASTM Customer Service at [service@astm.org](mailto:service@astm.org). For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

### 3.2.3.1 *Discussion*—

The term non-parameterized computer code refers to a generalized computer program in which values of parameters can be specified by the user.

3.2.4 *heat transport model, n*—in groundwater modeling, an application of a mathematical model to represent the movement of heat or energy in a groundwater system.

3.2.5 *inverse model, n*—in groundwater modeling, an application of a mathematical model designed for evaluating groundwater system parameters and stresses by minimizing the differences between computed and observed system responses.

### 3.2.5.1 *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 groundwater system. Aquifer test and tracer test analysis software are often based on analytical models of the groundwater system. Since they include automated procedures to estimate the system parameters, they can be considered *inverse* models.

3.2.6 *numerical model, n*—in groundwater modeling, a model that uses numerical/mathematical methods to solve the governing equations of the applicable problem.

3.2.7 *prediction model, n*—an application of a mathematical model designed for predicting groundwater 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.~~

#### 3.2.7.1 *Discussion*—

These models are based on a so-called forward or direct mathematical formulation of the physical processes.

3.2.8 *solute transport model, n*—~~an~~ in groundwater modeling, the application of a mathematical model to represent the movement of chemical species dissolved in groundwater.

## 4. Significance and Use

4.1 Groundwater modeling ~~has become~~ is an important methodology in support of the planning and decision-making processes involved in groundwater management. Groundwater models provide an analytical framework for obtaining an understanding of the mechanisms and controls of groundwater 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~~ needed and cost-effective support for planning and screening of alternative policies, regulations, and engineering designs affecting groundwater.<sup>3</sup>

4.2 There are many different groundwater 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~~ needed for the project.

4.3 In practice, it is often difficult to determine the capabilities, operational characteristics, and limitations of a particular groundwater 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.<sup>4</sup>

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 groundwater 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 groundwater modeling code through the formulation of a code classification system and the presentation of code description guidelines.

## 5. Classification of Groundwater Modeling Codes

5.1 There are many groundwater modeling codes available designed to simulate, describe, or analyze different types of groundwater systems and problems. The descriptive information of such software can be divided in three groups.<sup>5</sup>

5.1.1 *General Software Information*, 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*, 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 groundwater 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:<sup>5</sup>

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

5.2.2 The nature of the groundwater system that can be simulated with the software; and,

5.2.3 The mathematical framework.

5.3 *Objective-Oriented Classification*<sup>5</sup>(see **Table 1**):

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

<sup>3</sup> 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.

<sup>4</sup> 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~~ 1997.

<sup>5</sup> 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.

5.3.2 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 groundwater 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.

## iTeh Standards (<https://standards.itih.ai>) Document Preview

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TABLE 1 Classification Categories for Groundwater Modeling Software<sup>6</sup>

	Code Design Objectives
	<p>Applicability of the software to certain types of groundwater management problems</p> <p>Calculated variables:</p> <ul style="list-style-type: none"> <li>Screening/ranking</li> <li>Prediction</li> <li>Backtracking</li> <li>Inverse or parameter estimation</li> <li>Optimization</li> </ul> <p>Functional use:</p> <ul style="list-style-type: none"> <li>Research</li> <li>Education and demonstration</li> <li>General system characterization</li> <li>General engineering screening/design</li> <li>Site/problem dedicated</li> <li>Policy/strategy screening</li> </ul> <p>Nature of Groundwater System: Hydrogeological and Soil-Morphological Framework</p> <p>Hydrostratigraphy:</p> <ul style="list-style-type: none"> <li>Water-saturated versus partially saturated</li> <li>Porous medium versus fractured rock</li> <li>Single, simple system versus multilayered system of aquifers and aquitards or soils</li> <li>(Leaky-) confined versus phreatic aquifer conditions</li> <li>Heterogeneity, anisotropy</li> </ul> <p>Boundaries and internal geometry</p> <ul style="list-style-type: none"> <li>System boundaries: location and conditions (for example, recharge; groundwater divide; impermeable base; stream; pond; seepage face; springs; point, line, or patch contaminant or heat source; diffuse source, and so forth)</li> <li>Model layers</li> <li>Internal discontinuities (faults)</li> </ul> <p>Simulation scale:</p> <ul style="list-style-type: none"> <li>Laboratory scale</li> <li>Experimental field scale</li> <li>Local or site scale</li> <li>Regional or basin scale</li> </ul> <p>Fluid conditions:</p> <ul style="list-style-type: none"> <li>Type of fluid (water, NAPL, vapor, steam)</li> <li>Varying versus constant fluid viscosity</li> <li>Varying versus constant fluid density</li> <li>Compressible versus noncompressible fluid</li> </ul> <p>Nature of Groundwater System: Physical, Chemical, and Biological Processes</p> <p>Flow type:</p> <ul style="list-style-type: none"> <li>Saturated flow</li> <li>Unsaturated flow</li> <li>Vapor transport</li> <li>Multiphase flow (water/air or vapor; water/NAPL; water/steam; salt water/fresh water)</li> </ul> <p>Flow conditions:</p> <ul style="list-style-type: none"> <li>Laminar versus turbulent</li> <li>Steady-state versus time-varying conditions</li> </ul> <p>Phase changes</p> <p>Chemical transport:</p> <ul style="list-style-type: none"> <li>Nonreactive soluble species</li> <li>Reactive soluble species</li> <li>Facilitated transport</li> <li>Vapor phase transport</li> <li>(Bio-) chemical transformations</li> <li>Interphase transfers</li> <li>Heat transport</li> <li>Biota transport (bacteria and viruses)</li> <li>Matrix deformation due to fluid injection or withdrawal</li> <li>Coupling with external systems (for example, surface water, plant uptake, atmosphere)</li> </ul> <p>Mathematical Framework</p> <p>General nature of equation:</p> <ul style="list-style-type: none"> <li>Empirical versus mechanistic</li> <li>Deterministic versus stochastic</li> <li>Lumped versus distributed</li> </ul>

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Dimensionality of equations (1D, 2D, 3D, steady-state, transient)  
 Type of boundary condition (first, second, third; flow, transport)  
 Solution method:  
 Analytical (single solution, superposition, semi-analytical solution, analytic element method)  
 Numerical:  
 Spatial approximation (finite difference method, finite element method, boundary element method, path line integration, method of characteristics, random walk method)  
 Time-stepping scheme  
 Matrix solution technique

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5.3.4.4 *Inverse or Parameter Estimation Models*—Evaluating system parameters when a history of stresses and responses for the system are known from observation; inverse models are designed to determine the most likely distribution of system and process parameters such as, hydraulic parameters, transmissivity, leakage factor, storage coefficient, dispersivity, retardation coefficient, and so forth.

5.3.4.5 *Optimization Models*—Determining optimum location of sources and sinks and other management strategy-related, variable modeling features using mathematical optimization techniques. In this type of model, the hydrologic system is described in terms of objective function(s) and constraints representing management strategies. In groundwater modeling, models based on the use of optimization techniques are sometimes called management models.

5.4 *Classification Based on the Nature of the Groundwater System*<sup>5</sup>(see [Table 1](#)):

5.4.1 The nature of a groundwater system can be described in terms of the system’s hydrogeological and soil-morphological framework; the fluid conditions present; and the physical, chemical, and biological processes that take place.

5.4.2 The hydrogeological and soil-morphological framework includes:

5.4.2.1 *Hydrostratigraphy*—Includes saturated versus unsaturated conditions, aquifer and aquitard distribution; porous medium or fractured medium, or both; degree of heterogeneity and anisotropy;

5.4.2.2 *Simulation Scale*—Includes laboratory scale, experimental field scale, local or site scale, regional or basin scale; level of parameter and stress aggregation; and sometimes model formulation are a function of scale;

5.4.2.3 *Boundaries and Internal Geometry*—These include, but are not limited to, boundary location and conditions, model layers, and internal discontinuities such as faults and artificial barriers;

5.4.2.4 *Fluid Types*—Commonly, one of the fluids is water. Sometimes the fluid is a vapor mixture of water, air, and one or more volatile organic compounds (VOCs). If more than one fluid is present, the nonaqueous fluid can be air, methane, or another vapor, or it can be an immiscible nonaqueous phase liquid (NAPL); and

5.4.2.5 *Fluid Properties*—Fluid properties may vary in space or change in time, or both. Typically, fluid properties subject to such variability include density and viscosity, for example, as a function of concentration of dissolved constituents or temperature, or both. When NAPLs are present in groundwater, its density compared with that of water is of importance, for example, light NAPL or LNAPL—density is less than that of water; dense NAPL or DNAPL—density is more than that of water. A further distinction can be made in the modeling of condensable gases, for example, water vapor, and noncondensable gases, for example, air.

5.4.3 Relevant processes in groundwater modeling include the following (see [Table 2](#) for details):

5.4.3.1 Fluid flow (flow type and flow conditions);

5.4.3.2 Phase changes;

5.4.3.3 Chemical transport;

5.4.3.4 (Bio-)chemical transformations;

5.4.3.5 Heat transport;

5.4.3.6 Biota transport (bacteria and viruses);

5.4.3.7 Matrix deformation; and

5.4.3.8 Interaction processes with external systems, for example, atmosphere, plants, surface water.

5.4.4 *Fluid Flow*—refers to the movement of one or more fluids in porous or fractured rock:

5.4.4.1 In case the model fluid is water, a distinction is made between flow in a fully water saturated medium, that is, saturated flow, and flow in a medium that is only partially filled with water, that is, unsaturated flow or variably saturated flow. Some models can handle the change in time from fully saturated to partially saturated conditions and the reverse.

5.4.4.2 When, in addition to water, when other immiscible fluids are present, the system may be modeled as a multi-phase flow or multi-fluid flow problem (for example, flow of water and air or vapor, flow of water and NAPL). The term multi-phase flow also applies when water moves in two distinct phases, especially in liquid form and steam or vapor.

5.4.4.3 A special case of multifluid flow is encountered in sea-water intrusion modeling. In this case, the properties (density and viscosity) of a single fluid flow (water) may vary spatially. For example, such a situation is present when layers of water of distinct density are separated by a relatively small transition zone (salt/fresh water interface) and do not mix on the time scale of the simulation. The flow in the two layers may be simulated separately, coupled by boundary conditions at the interface. Occasionally, one of the layers (or fluids) may be considered stagnant, typically, the denser layer.