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Standard Guide for
Describing the Functionality of a Ground-Water Modeling Code[1]

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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 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 Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application[2]

D 5718 Guide for Documenting a Ground-Water Flow Model Application[2]

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[1] This guide is under the jurisdiction of ASTM Committee D18 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. 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 groundwater 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. Groundwater 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.[3]

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.[4]

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

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[3] 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.

[4] 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.

ground-water modeling code through the formulation of a code 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.[5]

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:[5]

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*[5] *(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 Software[6]

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)

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[5] 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.

- Model layers
- Internal discontinuities (faults)

- Simulation scale:
  - Laboratory scale
  - Experimental field scale
  - Local or site scale
  - Regional or basin scale
- Fluid conditions:
  - Type of fluid (water, NAPL, vapor, steam)
  - Varying versus constant fluid viscosity
  - Varying versus constant fluid density
  - Compressible versus noncompressible fluid

Nature of Ground-Water System: Physical, Chemical, and Biological Processes

- Flow type:
  - Saturated flow
  - Unsaturated flow
  - Vapor transport
  - Multiphase flow (water/air or vapor; water/NAPL; water/steam; salt water/fresh water
- Flow conditions:
  - Laminar versus turbulent
  - Steady-state versus time-varying conditions
- Phase changes
- Chemical transport:
  - Nonreactive soluble species
  - Reactive soluble species
  - Facilitated transport
  - Vapor phase transport
  - (Bio-) chemical transformations
  - Interphase transfers
  - Heat transport
  - Biota transport (bacteria and viruses)
  - Matrix deformation due to fluid injection or withdrawal
  - Coupling with external systems (for example, surface water, plant uptake, atmosphere)

Mathematical Framework

- General nature of equation:
  - Empirical versus mechanistic
  - Deterministic versus stochastic
  - Lumped versus distributed
- 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

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 ground-water modeling, models based on the use of optimization techniques are sometimes called management models.

5.4 *Classification Based on the Nature of the Ground-Water System*[5] *(see Table 1):*

5.4.1 The nature of a ground-water 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 ground water, 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 ground-water 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.

TABLE 2 Important Physical and Chemical Processes in Ground-Water Systems[6]

- Flow Processes:
  - Single fluid flow
  - Multifluid flow:
    - Multicomponent
    - Multiphase
  - Laminar flow:
    - Linear/Darcian
    - Nonlinear/non-Darcian
  - Turbulent flow
- Transport Processes:
  - Advection/convection
  - Conduction (heat)
  - Mechanical/thermal dispersion
  - Molecular diffusion
  - Radiation (heat)
- Transformation Processes:
  - Hydrolysis/substitution
  - Dissolution/precipitation
  - Oxidation/reduction
  - Complexation
  - Radioactive decay
  - Microbial decay/biotransformation
- Interphase Transfers:
  - Solid←→gas-(vapor) sorption
  - Solid←→liquid:-sorption ion exchange
  - Liquid←→gas-volatilization:
    - Condensation
    - Sublimation
- Phase Changes:
  - Freezing/thawing
  - Vaporization (evaporation)/condensation
- Matrix Deformation:
  - Compaction
  - Expansion
  - Fracturization

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.

5.4.4.4 Some modeling codes are designed specifically for simulation of vapor transport problems, for example, for use in the design of vapor extraction systems. These models concern the flow of a single, some times highly compressible fluid.

5.4.4.5 In some cases, spatial and temporal differences in fluid properties have a significant effect on the distribution of the computed variables. This may be the result of changes in the distribution of chemical species or heat. The fluid properties affected include density, viscosity, and compressibility. In codes designed for such problems, the mathematical solution of the flow and transport equations are coupled.

5.4.5 *Phase Changes*—Under certain conditions, a fluid may exist within the model domain in more than one phase. In ground-water modeling, this is particularly the case when the fluid is water, which can be in the solid phase (ice), the liquid phase (water), and the gas phase (vapor or steam). Occasionally, a phase change takes place at the same time throughout the model domain. More often, different phases coexist within the model domain and distinct boundaries exist between the phases. Across such (possibly moving) phase boundaries a change of state takes place, for example, freezing, thawing, evaporation, condensation, sublimation, melting, and so forth. Typically, these types of physical phenomena are encountered when simulating geothermal reservoirs or flow and transport in soils subject to low temperatures. The recent interest in steam injection for remediation makes it a major application of the multiphase model with explicit phase transitions.

5.4.6 *Chemical Transport*—The distribution of chemicals in ground water is dependent on such factors as source history, background distribution, transport and transformation processes, phase changes, and interphase transfer of chemical compounds, for example, sorption between liquid and solid phase and between gas and solid phase. Various types of modeling approaches are used to evaluate the distribution of chemicals in ground water.

5.4.6.1 *Solute Transport Models*—Spatially distributed simulation of physical transport of (in water) dissolved chemicals or solutes; they also are referred to as mass transport models or solute migration models. Typically, such models compute the spatial and temporal distribution of one or more chemical species. A solute transport model requires velocities for the calculation of advective displacement and spreading by dispersion.

5.4.6.2 The spatially distributed simulation of physical transport of nonreactive dissolved chemicals or solutes is subject to conservation of mass in the dissolved phase only, that is, conservative solute transport. Typically, such models include a mathematical representation of fluid flow related movement (advective transport), mechanical dispersion, and molecular diffusion.

5.4.6.3 In the spatially distributed simulation of transport of reactive solutes, that is, nonconservative solute transport, a single equation represents the conservation of mass in the dissolved phase; fluid-flow-related movement (advective transport); mechanical dispersion; molecular diffusion; and the effects of interphase transfers (adsorption), transformation (first-order decay); and zero-order production (source/sink term). The inclusion of transformation processes often is based on the assumption that the reaction proceeds instantaneously to equilibrium conditions.

5.4.6.4 *Hydrogeochemical Specification Models or Local Thermodynamic Equilibrium (LTE) Models*—Spatially lumped simulation of chemical processes occurring in ground water, that is, equilibrium-based or kinetics-controlled processes, including transformation processes and interphase transfers.

The mathematical formulation does not include spatial distribution aspects and assumes complete and instantaneous mixing of reactive compounds within the simulated volume.

5.4.6.5 These models, which are general in nature and often used for both ground water and surface water, simulate chemical processes in the liquid phase and sometimes between the liquid and solid phase (precipitation-dissolution and sorption) that regulate the concentration of dissolved constituents. They can be used to identify the effects of temperature, speciation, sorption, and solubility on the concentrations of dissolved constituents.

5.4.6.6 *Biotransformation or Biodegradation Models*—Spatially lumped or distributed simulation of biochemical processes (aerobic and anaerobic), including chemical transformation and pollutant degradation processes. These models sometimes include the simulation of biota population dynamics. They are used to identify the effects of microbial processes and relevant environmental conditions on the concentrations of dissolved constituents.

5.4.6.7 Some chemical compounds are hydrophobic and are transported primarily in conjunction with carriers, such as colloids, that is, facilitated transport.

5.4.6.8 *Vapor-Phase Transport*—Refers to the displacement of chemical species as a component of soil vapor. Typically, vapor-phase transport concerns a single fluid flow approach to the movement of a volatile compound.

5.4.6.9 Coupled simulation of distributed transport and interphase transfer processes, that is, solute transport models and locally lumped transformation and interphase transfer processes, that is, geochemical speciation models, facilitate detailed analysis of the transformation processes taking place during the transport of a chemical compound or analysis of the interaction of multiple chemical compounds in a moving fluid system.

5.4.6.10 Coupled simulation of distributed transport and interphase transfer processes and locally lumped biotransformation and biodegradation processes facilitate detailed analysis of the chemical transformations taking place during the transport of a chemical compound due to microbial activity and analysis of the influence of supporting chemical compounds on the efficiency of the transformation processes.

5.4.7 *Heat transport models*—concern with the displacement of energy or heat in the subsurface. There are three major types of heat transport models in the subsurface:

5.4.7.1 Transport through the fluid phase of the subsurface only, for example, water or air;

5.4.7.2 Transport through the solid phase of the subsurface only, for example, in dry rock; and,

5.4.7.3 Transport through both the fluid and solid phases of the subsurface.

5.4.7.4 In ground-water modeling only model types 5.4.7.1 and 5.4.7.2 are used. Within each of these two groups of models one can distinguish four subtypes:

(*a*) Low-temperature, single-phase heat transport without phase change, for example, to evaluate heat-pump efficiencies;

(*b*) Low-temperature, dual-phase heat transport with two fluids (water and vapor, for example, in soils);

(*c*) Low-temperature, dual-phase heat transport with phase change (freezing/thawing, for example, for studying frost front propagation in soils); and

(*d*) High-temperature, multiphase (liquid/vapor) heat transport with phase change (steam/water, for example, for evaluation of geothermal exploration potential).

5.4.7.5 Typical processes incorporated in heat transport models are convection, thermal dispersion, thermal conduction, and radiation. Some more complex models include evaporation/condensation and fluid-to-solid heat transport.

5.4.8 *Biota transport*—concern with the movement and fate of living organisms in ground-water systems, specifically bacteria and viruses. The concern with viruses in ground water is directly related to the potential health hazard they may pose. Bacteria transport is of interest for both health-risk reasons and in situ bioremediation of certain types of contamination. Although invertebrates, for example, crayfish, and small vertebrates, for example, small fish, may occur in (karstic) ground-water systems, thus far, the movement of these species in ground-water systems has not been modeled.

5.4.9 *Matrix deformation*—refers to displacements and deformation of the solid phase of a porous or fractured medium. Such deformation may be due to natural causes, for example, stress release from erosion, stress increase from sediment deposition, and stress changes from earthquake vibration, or manmade, for example, injection or removal of fluids and vibration or shock waves. In ground-water modeling, matrix deformation typically results from induced changes in fluid pressure. Simple models calculate the resulting change in land elevation only. More complex models may couple the flow model with a multidimensional geomechanical model to include the effects of changes in the matrix on flow parameters, for example, hydraulic conductivity and storativity, accounting for heterogeneity. Occasionally, flow and matrix deformation models are coupled with a heat-transport model to account for the effects of temperature changes on the rock matrix displacement.

5.4.10 Many models address the interaction between ground water and the other components of the hydrologic cycle. Most of these models describe only the inputs and outputs at interfaces with other components of the hydrologic cycle as dynamic stresses or boundary conditions. Increasingly, models have been developed which simulate the processes in each subsystem in detail and on an appropriate time scale, resulting in comprehensive hydrologic models. The most common interaction models include the simulation of surface runoff and stream flow, (for example, watershed models and stream-aquifer models), the loss of water from the subsoil to the atmosphere (evapotranspiration), and the removal of water and solutes by plants (plant uptake).

5.5 *Classification Based on Mathematical Approaches*[5] *(see Table 1)*:

5.5.1 There are three main categories of characteristics for describing the mathematical framework of ground-water models: the general nature of the governing equations and implemented boundary conditions; the dimensionality in the space and times domain (for variables, parameters, and boundary conditions); and the solution method(s) employed. Documentation of a ground-water model should include the governing equations(s) and the boundary and initial conditions in mathematical form together with a complete list of variables used in the equations.

5.5.2 *Nature of the Governing Equations*—The governing equations represent the understanding of the nature of the processes considered important to the problem at hand. In ground-water modeling, three types of models can be distinguished based on the nature of the mathematical representation of the ground-water system in the form of governing equations as follows:

5.5.2.1 *Lumped-Parameter Models*, based on calibrated transfer functions (black box models) representing the cause-and-effect or input-response relationships for the studied system. Lumped parameter models assume that a system may be defined with a single, non-spatially distributed value for the primary system variables. The system's input-response function does not necessarily reflect known physical laws and the system parameters do not necessarily represent physical parameters;

5.5.2.2 *Deterministic Distributed-Parameter Models*, based on precise, mechanistic, process-based descriptions of cause-and-effect or input-response relationships. The responses are presented as a single spatial and temporal distribution of the dependent variable; and

5.5.2.3 *Stochastic Distributed-Parameter Models*, reflecting the probabilistic or stochastic nature of a ground-water system in describing the spatial and temporal variability of relevant geologic, hydrologic, and chemical characteristics. The responses are presented as a stochastic distribution of the dependent variable for each location or time step, or both.

5.5.3 *Boundary Conditions*—Most ground-water modeling codes are based on mechanistic, process-based descriptions of the ground-water system. The complete mathematical statement using this equation formulation approach includes the definition of boundary conditions. Typically, there are up to three types of boundary conditions in groundwater models:

5.5.3.1 Boundary condition of the first kind or Dirichlet condition specifying the values of a dependent variable as a function of location, and possibly time, for example, prescribed pressure, head, water content, temperature, or concentration;

5.5.3.2 Boundary condition of the second kind or Neumann condition specifying the gradient of the dependent variable normal to the boundary as a function of location, and possibly time, for example, prescribed water flux, solute flux, or heat flux; and,

5.5.3.3 Boundary condition of the third kind, mixed condition, or Cauchy condition specifying the relationship between the state variable and its derivatives as a function of location, and possibly time, for example, at a leaky flow boundary or at the surface of a soil subject to infiltration in the presence of a gravity term.

NOTE 1—In saturated flow, two special cases of boundary conditions exist: free surface condition with or without accretion, and seepage surface. In both cases, the boundary condition is known, but the location of the boundary is either a priori unknown or partially defined and needs to be found as part of the mathematical solution.

NOTE 2—The type of boundary condition may vary along the boundary as well as in time.

5.5.4 *Dimensionality*:

5.5.4.1 In terms of spatial dimensionality, ground-water modeling codes may be capable of simulating systems in one, two, or three dimensions using Cartesian or axisymmetric coordinate systems and Eulerian, Lagrangian, or combined Eulerian-Lagrangian spatial definitions.

5.5.4.2 In the time domain, ground-water modeling codes may handle either transient, steady-state, or quasi-steady-state (successive steady-states) simulations, or combinations thereof.

5.5.5 *Solution Method Employed*—The governing equations for ground-water systems usually are solved either analytically or numerically.

5.5.5.1 Analytical models contain a closed-form (explicit) or analytical solution of the governing equation for specific initial and boundary conditions. Analytical solutions are continuous in space and time. Because of the complex nature of ground-water systems, analytical solutions only are available for a set of equations, initial conditions, and boundary conditions that represents a highly simplified conceptualization of the nature of the ground-water system.

NOTE 3—When the governing equations of selected subsets of the ground-water system approximately are linear in terms of the dependent variable, a solution may be derived by superposition of the (analytical) solutions of these equations describing a more complex representation of the ground-water system, resulting in superposition models. Specifically, the analytic element method is representative for this type of model.

NOTE 4—Often, complex analytical solutions require approximation in space or time, or both, by numerical techniques. Models based on this approach may be considered as semi-analytical or quasi-analytical. Models based on a closed-form solution for either the space or time domain, and which contain additional numerical approximations for the other domain, also are considered semi-analytical models. An example of the semi-analytic approach is the use of numerical integration to solve analytical expressions for streamlines or for certain solute transport problems.

5.5.5.2 In numerical models, a discrete solution is obtained in both the space and time domains by using numerical approximations of the governing (partial) differential equation based on discretization of the space and time domains. As a result of these approximations, the conservation of mass is not always ensured, because of truncation and rounding errors, and thus, needs to be verified for each application.

NOTE 5—Conservation of mass in a discrete solution does not guarantee a particular accuracy level. Spatial and temporal resolution in applying, such models, is a function of study objectives and availability of data. Accuracy is a function of spatial and temporal discretization and numerical solution parameters, among others.

5.5.5.3 Various discrete solution techniques are used in ground-water models. They include finite-difference methods (FD), integral finite-difference methods (IFDM), Galerkin and variational finite-element methods (FE), collocation methods, boundary (integral) element methods (BIEM or BEM), particle mass tracking methods such as random walk (RW), and the method of characteristics (MOC).

5.5.5.4 Most numerical methods result in a set of algebraic equations, which are solved using direct or iterative matrix methods.

5.5.5.5 Many of the numerical codes for transport modeling in ground-water solve for the flow equation and one or more transport equations. The flow and transport solution are called *linked* when the code first computes the flow solution for each time step, independently from the transport solution at any time. When the solution of the transport equation influences the solution of the flow equation, such as is the case.

6. Functionality Description

6.1 Functionality description involves the identification and description of the functions of a simulation code in terms of model framework geometry, simulated processes, boundary conditions, and analytical capabilities. The functions of the code are grouped and described systematically using a set of standard descriptors[4] (see Table 3). If necessary, the list of descriptors may be adapted or expended to cover features resulting from new research or software development progress.

6.2 The documentation of a ground-water modeling code should include a section called "Functionality Description" or" Code Functions and Capabilities" that addresses all pertinent descriptors from Table 3. This section also should include additional details where the descriptors of Table 3 are insufficient to describe all features and capabilities of the code.

6.3 Table 3 can be used as a checklist if in reviewing a code for potential use in a project, the documentation of the code does not contain a section describing the code's functionality in sufficient detail.

6.4 Table 3 also can be used for determining project needs as part of a code selection process. The code selection process in ground-water modeling is described in separate guides, for example, Guide D 5447.

TABLE 3 Functionality Descriptors

Type of Information	Comments
General Software Information[5]	
Software identification number	unique number, for example a data base key number
Software name	acronym; full name in brackets; if no name known provide short description
Description date	date when description was prepared
Functionality description analyst	name of person who prepared this description
Date of first release of software	
Version number of latest (current) release	
Date of latest release	official software release date by custodian, latest date or documentation, latest date stamp on program files
Name of authors of code	last name first followed by initials for first author (to allow sorting by latest name of principal author), other authors start with initials followed by last name; no institution names in this field (see separate field)
Development purpose/objective	see Table 1
System(s) of supported units	units of measurement
Short description of model	abstract/summary; should include aspects of hydrogeology, dimensionality, transient/steady-state, flow and transport processes, boundary conditions, mathematical methods, calculated variables, user-interface, output options, and so forth
Computer system requirements	list requirements per computer platform separated by commas; list different platforms separated by semicolons; include hardware and software requirements
Program code information	language, compiler, and so forth; reviewer's compilation information if code is received in uncompiled form
Description of documentation	concepts and theory, test results, model setup advice, input instructions, example problems, program flow chart, code/modules description (function, design), code structure, installation/compilation instructions, and so forth
Evaluation of documented code testing	describe what kind of testing has been performed
Evaluation of level of external review	refers to description of theoretical framework, code performance, and other issues in peer-reviewed journals, reports, or textbooks
Code input processing capabilities	code input preparation, data editing, type of user-interface (for example, graphic user interface, inport of site maps, and grid design options), file import capabilities (file formats)
Code output processing capabilities	form of screen output (for parameter/variable type see specific software types); file save and export options
Code operation	batch operation, operation from menu-based shell, user-interactive computational features
Code availability terms	public domain, proprietary, licensed, copyrighted, share-ware, and so forth
Availability of software support	type, level, and conditions; identify source of support in terms of custodian, distributor, or other parties
Development institution	name and address of institute, university/department, agency/department, or company where code has been developed
Custodian institution	name and address of institute, university/department, agency/department, or company which is responsible for code maintenance
Physical Framework[5]	
Spatial dimensionality and temporal characteristics	spatial dimensions and time stepping supported by code
Characteristics of numerical grid	fixed versus flexible number of cells/elements, size/shape of cells/elements, fixed versus movable grids, manual versus automatic grid generation, and so forth
Hydrostratigraphic characteristics	type of aquifers, sequence of aquifers/aquitards, soil-layering, porous versus fractured medium, representation of fractures, anisotropy, level of heterogeneity, perched water tables, macropores
Geometry	regular versus irregular external boundaries, orientation of layer boundaries, location and shape of internal boundaries, presence of internal discontinuities
Medium properties	parameter distribution in time and space supported by code
Flow Simulation Capabilities[4]	
Flow characteristics of saturated/unsaturated zone	for example, steady-state, transient, Darcian, turbulent, nonlinear laminar
Flow processes in saturated/unsaturated zone	for example, evaporation, condensation, evapotranspiration, recharge from precipitation, induced recharge, delayed yield from storage, infiltration, plant uptake, hysteresis, capillary rise

TABLE 3 *Continued*

Type of Information	Comments
Changing aquifer conditions	for example, soil layer/aquifer/aquitard pinch-out, storativity conversion in space/time (confined-unconfined),
Soil functions	soil characteristic function, hysteresis
Fluid conditions	water, vapor, water and air, water and NAPL or vapor, or combination thereof, steam and water, salt and fresh water (sharp interface), (in)compressible fluid, variable density, variable viscosity
Boundary/initial conditions for flow	see functionality descriptors for heat transport capabilities
Mathematical solution method(s) for flow part	analytical/approximate analytical/numerical solution; major numerical method, for example, analytic element, finite difference, integral finite difference, finite element; time discretization method; matrix solving technique(s)
Parameter identification for flow part of code	identified parameters, for example, recharge, hydraulic conductivity; identification method, for example, graphic curve matching, direct/indirect numerical method, linear/nonlinear regression, least squares
Output options for flow	for example, head/pressure, potential, drawdown, moisture content, intercell fluxes, velocities, stream function values, streamlines, path lines, traveltimes, isochrones, interface position, capture zone delineation, position saltwater wedge, water budget components (global water balance), boundary fluxes
Solute Transport Simulation Capabilities[5]	
Compounds model can handle	for example, any constituent, single constituent, two/more interacting constituents, TDS, heavy metals, nitrogen/phosphorus compounds, organics, radionuclides, bacteries, viruses
Transport and fate processes	for example, advection, mechanical dispersion, molecular diffusion, ion exchange, substitution, hydrolysis, dissolution, precipitation, redox reactions, acid/base reactions, complexation, radioactive decay, chain decay, first-order (bio-) chemical decay, aerobic/anaerobic biotransformation, plant solute uptake, vapor phase sorption, liquid phase sorption (linear isotherm/retardation, Langmuir/Freundlich isotherm, sorption hysteresis, nonequilibrium sorption), volatilization, condensation, (de)nitrification, nitrogen cycling, phosphorus cycling, die-off (bacteries, viruses), filtration
Boundary/initial conditions for solute transport	for example, fixed concentration or specified time-varying concentration, zero solute flux, fixed or specified time-varying cross-boundary solute flux, solute flux from stream dependent on flow rate and concentration in stream, solute flux to stream dependent on flow rate and concentration in ground-water, injection well with constant or specified time-varying concentration and flow rate, production well with solute flux dependent on concentration in ground-water, solute flux dependent on intensity and concentration of natural recharge
Mathematical solution method(s) for solute transport part of code	coupling with fluid flow (concentration-influenced density and viscosity); analytical/approximate analytical/ numerical solution; major numerical method, for example, analytic element, finite difference, integral finite difference, finite element, method of characteristics, random walk method; time discretization method; matrix solving technique(s)
Output options for solute transport	type of output, for example, concentration values, concentration in pumping wells, internal and cross-boundary solute fluxes, mass balance components (cell-by-cell, global), uncertainty in results (that is, statistical measures); form of output, for example, results in ASCII text format, spatial distribution and time series of concentration for post-processing, direct-screen display (text, graphics), and graphic vector file (HGL, DXE) or graphic bitmap/pixel/raster file (BMP, PCX, TIF); computational progress, for example, iteration progress and error, mass balance error, cpu use, and memory allocation
Heat Transport Simulation Capabilities[5]	
Heat transport processes	for example, convection, rock matrix conduction, fluid conduction, thermal dispersion, thermal diffusion (into aquifer matrix), thermal expansion of liquid, radiation, phase changes (water-steam, water-ice), evaporation, condensation, freezing/thawing
Boundary/initial conditions for heat transport	for example, fixed or specified time-varying temperature, zero heat flux, fixed or specified time-varying cross-boundary heat flux, injection well with constant or specified time-varying temperature and flow rate, production well with heat flux dependent on temperature of ground-water, heat flux dependent on intensity and temperature of natural recharge
Mathematical solution method(s) for heat transport part of code	coupling with fluid flow; temperature-influenced density and viscosity; modification of hydraulic conductivity; analytical/approximate analytical/numerical solution; major numerical method, for example, analytic element, finite difference, integral finite difference, finite element, method of characteristics, random walk method; time discretization method; matrix solving technique(s)
Output options for heat transport	type of output, for example, temperature values, temperature in pumping wells, internal and cross-boundary heat fluxes, heat balance components (cell-by-cell, global), uncertainty in results (that is, statistical measures); form of output, for example, results in ASCII text format, spatial distribution and time series of temperature for post-processing, direct-screen display (text, graphics), and graphic vector file (HGL, DXF) or graphic bitmap/pixel/raster file (BMP, PCX, TIF); computational progress, for example, iteration progress and error, heat/energy balance error, cpu use, and memory allocation
Capabilities Regarding Simulation of Rock Matrix Deformation[5]	
Deformation cause	for example, fluid withdrawal (increased internal rock stresses), overburden increase (increased system loading), manmade cavities and karst cave-in (reduced rock stresses)
Deformation model components	for example, displacements in aquifer, aquitard, or overburden, or combination thereof
Type of deformation model	for example, empirical relationship, depth/porosity model, aquitard drainage model, mechanistic model (process-based model)
Deformation processes	for example, subsidence (vertical movement of land surface), compaction/consolidation (vertical deformation, decrease of layer thickness), 2D/3D matrix deformation, matrix expansion (due to releases of skeletal stresses), coupling with fluid flow, parameter reestimation (calculating effects of deformation on hydraulic conductivity and storage coefficient), elastic/plastic deformation; stress-dependent hydraulic conductivity compressibility of rock matrix
Boundary/initial conditions deformation	for example, prescribed constant or time-varying displacement, prescribed pore pressure, prescribed skeletal stress
Mathematical solution method(s) for deformation	analytical/approximate analytical/numerical solution; major numerical method, for example, finite difference, integral finite difference, finite element, method of characteristics; time discretization method; matrix solving technique(s)

TABLE 3 *Continued*

Type of Information	Comments
Output options for deformation	type of output, for example, matrix displacements (internal skeletal displacements; 1D, 2D, 3D), surface displacements (subsidence; 1D), pore pressure, skeletal stress/strain, calculated parameters; uncertainty put, for example, results in ASCII text format, spatial distribution and time series of displacements, pore pressure or stress/strain for post-processing, direct-screen display (text, graphics), and graphic vector file (HGL, DXF) or graphic bitmap/pixel/raster file (BMP, PCX, TIF); computational progress, for example, iteration progress and error, cpu use, and memory allocation
Optimization of Management Decisions[5]	
Type of management model	for example, lumped parameter, distributed parameter
Objective function	for example, hydraulic objective function (heads, pumping rates), water quality objective function (concentrations, removed mass), economic objective function (cost)
Optimization constraints	for example, drawdown, pumping/injection rates, concentration at compliance point, removed mass (because of treatment/disposal)
Decision variables	for example, pumping/injection rates, cost
Mathematical solution method(s) for management model	for example, embedding method, linked simulation-optimization, response matrix method, hierarchical approach, Lagrangian multipliers, linear/quadratic/stochastic/mixed integer/dynamic programming
Output options for management model	for example, location of wells, pumping/injection rates

7. Keywords

7.1 code selection; ground-water; ground-water modeling; model types; software functionality