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Standard Guide for Subsurface Flow and Transport Modeling[1]

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1. Scope

1.1 This guide covers an overview of subsurface fluid-flow (ground-water) modeling. The term subsurface fluid flow is used to reduce misunderstanding regarding ground water, soil water, vapors including air in subsurface pores, and non-aqueous phase liquids. Increased understanding of fluid-flow phenomena is the combined result of field investigations and theoretical development of mathematical methods to describe the observations. The results are methods for modeling viscous fluids and air flow, in addition to water, that are practical and appropriate.

1.2 This guide includes many terms to assist the user in understanding the information presented here. A ground-water system (soils and water) may be represented by a physical, electrical, or mathematical model, as described in 6.4.3. This guide focuses on mathematical models. The term mathematical model is defined in 3.1.11; however, it will be most often used to refer to the subset of models requiring a computer.

1.3 This guide introduces topics for which other standards have been developed. The process of applying a ground-water flow model is described in Guide D 5447. The process includes defining boundary conditions (Guide D 5609), initial conditions (Guide D 5610), performing a sensitivity analysis (Guide D 5611), and documenting a flow model application (Guide D 5718). Other steps include developing a conceptual model and calibrating the model. As part of calibration, simulations are compared to site-specific information (Guide D 5490), such as water levels.

1.4 Model use and misuse, limitations, and sources of error in modeling are discussed in this standard. This guide does not endorse particular computer software or algorithms used in the modeling investigation. However, this guide does provide references to some particular codes that are representative of different types of models.

1.5 Typically, a computer model consists of two parts; computer code that is sometimes called the computer program or software, and a data set that constitutes the input parameters that make up the boundary and initial conditions, and medium and fluid properties. A standard has been developed to address evaluation of model codes (see Practice E 978).

1.6 Standards have been prepared to describe specific aspects of modeling, such as simulating subsurface air flow using ground-water flow modeling codes (see Guide D 5719) and modeling as part of the risk-based corrective action process applied at petroleum release sites (see Guide ES 38).

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 4105 Test Method (Analytical Procedure) for Determining Transmissivity and Storage Coefficient of Nonleaky Confined Aquifers by the Modified Theis Non-Equilibrium Method[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 to a Site-Specific Problem[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[3]

[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*, Vol04.09.

D 5719 Guide to Simulation of Subsurface Air Flow Using Ground-Water Flow Modeling Codes[3]

E 943 Terminology Relating to Biological Effects and Environmental Fate[4]

E 978 Practice for Evaluating Mathematical Models for the Environmental Fate Models of Chemicals[4]

ES 38 Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites[5]

3. Terminology

3.1 *Definitions:*

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

3.1.2 *boundary condition*—a mathematical expression of a state of the physical system that constrains the equations of the mathematical model.

3.1.3 *calibration (model application)*—the process of refining the model representation of the hydrogeologic framework, hydraulic properties, and boundary conditions to achieve a desired degree of correspondence between the model simulation and observations of the ground-water system.

3.1.4 *conceptual model*—an interpretation or working description of the characteristics and dynamics of the physical system.

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

3.1.6 *deterministic process*—a process in which there is an exact mathematical relationship between the independent and dependent variables in the system.

3.1.7 *fidelity*—the degree to which a model application is designed to be realistic.

3.1.8 *finite-difference method*—in *subsurface fluid flow*, a numerical technique for solving a system of equations using a rectangular mesh representing the aquifer and solving for the dependent variable in a piece wise manner.

3.1.9 *finite-element method*—in *subsurface fluid flow*, a numerical technique for solving a system of equations using an irregular triangular or quadrilateral mesh representing the aquifer and solving for the dependent variable in a continuous manner.

3.1.10 *ground-water flow model*—application of a mathematical model to represent a site-specific ground-water flow system.

3.1.11 *mathematical model*—mathematical equations expressing the physical system and including simplifying assumptions. The representation of a physical system by mathematical expressions from which the behavior of the system can be predicted.

3.1.12 *method of characteristics*—in *subsurface fluid flow*, a numerical method to solve solute transport equations by construction of an equivalent system of ordinary differential equations using moving particles as reference points. Also known as the particle-in-cell method.

3.1.13 *model*—an assembly of concepts in the form of mathematical equations that portray understanding of a natural phenomenon.

3.1.14 *numerical methods*—in *subsurface fluid flow modeling*, a set of procedures used to solve the equations of a mathematical model in which the applicable partial differential equations are replaced by a set of algebraic equations written in terms of discrete values of state variables at discrete points in space and time.

3.1.14.1 *Discussion*—There are many numerical methods. Those in common use in ground-water models are the finite-difference method, the finite-element method, the boundary element method, and the analytical element method.

3.1.15 *numerical model*—in *subsurface fluid flow modeling*, a model that uses numerical methods to solve the governing equations of the applicable problem.

3.1.16 *output*—in *subsurface fluid flow modeling*, all information that is produced by the computer code.

3.1.17 *random walk*—in *subsurface fluid flow modeling*, a method of tracking a large number of particles with the number of particles proportional to solute concentration, and each particle advected deterministically and dispersed probabilistically.

3.1.18 *sensitivity*—in *model application*, the degree to which the model result is affected by changes in a selected model input representing hydrogeologic framework, hydraulic properties, and boundary conditions.

3.1.19 *simulation*—in *ground-water flow modeling*, one complete execution of a ground-water modeling computer program, including input and output.

3.1.20 *sink*—in *subsurface fluid flow modeling*, a process whereby, or a feature from which, water is extracted from the ground-water flow system.

3.1.21 *steady-state flow*—a characteristic of a flow system where the magnitude and direction of specific discharge are constant in time at any point.

3.1.22 *stochastic*—in *subsurface fluid flow*, consideration of subsurface media and flow parameters as random variables.

3.1.23 *stochastic model*—in *subsurface fluid flow*, a model representing ground water parameters as random variables.

3.1.24 *stochastic process*—a process in which the dependent variable is random (so that prediction of its value depends on a set of underlying probabilities) and the outcome at any instant is not known with certainty.

3.2 For definitions of other terms used in this guide, see Terminology D 653 and Terminology E 943.

4. Summary of Guide

4.1 Modeling is a tool that can be used to evaluate many ground-water problems. Models are useful for reconnaissance studies preceding field investigations, for interpretive studies following the field program, and for predictive studies to estimate future field behavior. In addition to these applications, models are useful for studying various types of flow behavior by examining hypothetical aquifer problems.

4.2 Models can be described many different ways. In this guide they are differentiated by flow in porous versus karst or

[4] *Annual Book of ASTM Standards*, Vol 11.05.

[5] Discontinued; see *1994 Annual Book of ASTM Standards*, Vol 11.04.

fractured media, flow in single or multiphase, function, fidelity, construction, and method of solution.

5. Significance and Use

5.1 Subsurface fluid flow modeling is a well established tool that can aid in studying and solving soil and ground-water problems.

5.2 Evaluation of more complex problems has been allowed as a result of advances in computing power and numerical analysis, yet confusion and misunderstanding over application of models still exists. As a result, some inappropriate use occurs and some problems which could be readily addressed are not.

5.3 The purposes of this guide are to introduce the basic concepts of subsurface fluids modeling and to show how models are described and categorized.

5.4 This guide should be used by practicing ground-water modelers, purchasers of modeling services, and by those wishing to understand modeling.

6. Model Types

6.1 Simulation of a ground-water system refers to the construction and operation of a model whose behavior approximates the actual aquifer behavior. Models can be described in many different ways. Model description in this guide provides logical groupings to illustrate similarities and differences between models.

6.2 Models of subsurface flow can first be segregated into flow in porous medium flow and non-continuum (fractured and karst) flow. Flow can then be subdivided into single phase and multiphase flow. Single phase flow includes flow of water in the unsaturated and saturated zone. Multiphase flow includes unsaturated zone flow where water and air that occupy the pores flow independently or where two or more immisible fluids flow independently. Models of subsurface fluid flow then can be further subdivided for handling special cases, such as variable density of the fluid.

6.3 Most modeling is performed using porous medium flow codes where the governing equations are based on Darcy's law. In some settings and for some problems, flow through fractures may be represented with equivalent porous media behavior, however, the modeler must evaluate whether this is appropriate because of the fundamental difference between the mathematical model and the real system. This is considered further in 6.4.2.

6.4 For the purposes of this overview, models are classified according to their function, fidelity, construction, and mathematical method.

6.4.1 *Model Processes*—Four general types of models exist for the majority of problems: fluid flow, solute (contaminant) transport, heat transport, and deformation **(1)**.[6]

6.4.1.1 *Fluid Flow*—A fluid-flow model is normally described by one equation, usually in terms of hydraulic head, pressure, or potential. In multiphase flow, one equation is used for each phase. Ground-water flow models are often used to solve problems concerning water supply, ground-water/surface water interactions, capture zones, and dewatering.

6.4.1.2 *Solute Transport*—Solute transport is simulated with an equation in addition to the flow equation to solve for concentrations of the chemical species. Solute transport models are often used to solve problems concerning aquifer restoration, waste injection, sea-water intrusion, and underground storage tank releases.

6.4.1.3 Models have been developed to describe chemical transformations due to interactions between the fluid(s) composition and media composition. These models, called hydrogeochemical models, do not consider the transport processes, and can be subdivided into three major categories: thermodynamic codes, distribution-of-species codes, and reaction progress codes **(2)**. Several geochemical codes have been described by van der Heijde and Einawawy **(3)**.

6.4.1.4 *Heat Transport*—In a simple form heat flow is simulated with an equation in addition to the ground-water flow equation, similar to the solute transport equation, but in terms of temperature. In a more rigorous manner, heat flow is coupled with fluid flow. The equation for fluid flow must account for variable density and an additional equation is required to represent conduction of heat through the rock and its pores. Heat transport models are often used to solve problems with thermal storage, and thermal pollution. For evaluating geothermal energy development multiphase flow equations are required to consider the presence of water and steam.

6.4.1.5 *Deformation*—Aquifer deformation is simulated by combining a ground-water flow model with a set of equations that describes the stress/strain relation of the soil and rock media. Deformation models are often used to solve problems with land subsidence, soil settlement, or compaction.

6.4.2 *Model Fidelity*—Three general classifications of realism are described; screening, engineering calculation, and aquifer simulator **(4)**.

6.4.2.1 *Screening*—A screening model is least representative of the real system and is used to assess generalities and functions of processes. These applications may be useful with a low degree of correspondence between the simulation and the physical hydrogeologic system. Typical uses of screening model applications include assessing the qualitative behavior of the physical hydrogeologic system, identifying data collection needs, and conceptual designs for feasibility studies. Screening models may be used with "conservative" or "worst case" input parameters for gross differentiation or elimination of alternatives.

6.4.2.2 *Engineering Calculation*—Applications which are designed to predict the response of the physical hydrogeologic system to a specific change or family of changes in boundary conditions, hydrologic stresses, or aquifer parameters. These applications do not necessarily require a high degree of correspondence between the simulation and the physical hydrogeologic system because aspects of the model which are unrealistic may be designed to be conservative with respect to the intended use. Typical uses of engineering calculation applications include assessing a problem where dewatering to

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