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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[2]

D 5719 Guide to Simulation of Subsurface Air Flow Using Ground-Water Flow Modeling Codes[2]

E 943 Terminology Relating to Biological Effects and Environmental Fate[3]

E 978 Practice for Evaluating Mathematical Models for the Environmental Fate Models of Chemicals[3]

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

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

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

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ES 38 Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites[4]

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 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

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

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)**.[5]

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 achieve or exceed a certain elevation is required and ground-water capture of a solute is required rather than achievement of a specific concentration.

6.4.2.3 *Aquifer Simulator*—This is most representative of the real system and is used to assess the value of unknowns at specific locations and times. These applications require a high degree of correspondence between the simulation and the physical hydrogeologic system.

6.4.2.4 *Model Construction*—The model can be physical,

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

electrical analog, or computer code.

6.4.2.5 *Physical Models*—Physical models include sand tanks. Sand tank models are most commonly used as teaching tools and for demonstrations. They are not commonly used beyond demonstrations because of the difficulty of constructing a model that is representative of a field condition.

6.4.2.6 *Analog Models*—Analog models include resistor/capacitor networks to electrically simulate ground-water potentials **(5)**. With the advent of microcomputers, electric analog models are no longer used, in part, because of the labor requirements to construct and modify the model.

6.4.2.7 *Computer Codes*—Computer codes include a set of equations with specific assumptions to describe the physical processes active in the subsurface.

6.4.3 *Model Formulation*—A mathematical model may be deterministic, statistical, or a combination of the two.

6.4.3.1 *Deterministic Models*—Deterministic models include those with precisely defined parameters and exact expressions yielding one result.

6.4.3.2 *Statistical Models*—Statistical models, also called stochastic models, use multiple simulations with randomly varied input based on a specified distribution for selected input parameters. Statistical methods are useful in performing uncertainty analyses, classifying data, and describing poorly understood systems **(1)**. Rather than a single answer that results from a deterministic model, a stochastic model provides a range of answers that can be expressed through a probability distribution function **(6)**.

6.4.3.3 *Mathematical Model*—A mathematical model of any physical system begins with an understanding of the physical behavior of the system. A relationship between cause and effect is used to construct a conceptual model of how the system operates. For ground-water flow, these relationships are generally well known, and are expressed using concepts such as hydraulic gradient to indicate flow direction in an isotropic medium. For the movement of contaminants, either dissolved or free-phase, these relationships, especially those involving physical-chemical behavior, are less well understood. Transformation of the physics into mathematical terms, making appropriate simplifying assumptions, and developing governing equations is creation of the mathematical model.

6.4.3.4 Most mathematical models use one of two general approaches to solve the governing differential equations; analytical and numerical. The boundary integral method is a combination of analytical and numerical methods and the analytic element method is an elaborate analytical method.

6.4.3.5 If the equations are amenable to analytical solution, they are referred to as analytical models. The familiar Theis equation **(7)** represents the solution of one such analytical model (see Test Method D 4105). The greatest strength of the analytical methods lies in their capability in many cases to produce exact solutions to a flow or transport problem in terms of the controlling parameters **(8)**. This makes them valuable in checking the accuracy of numerical models which are subject to errors that are insignificant in analytical models (see Section 8).

6.4.3.6 *Numerical Models*—For more complex physical settings, where partial differential equations are best solved using numerical approximations, these approximations are called numerical models. Numerical models are most appropriate for general problems involving aquifers having irregular boundaries, heterogeneities, or spatially or time variant pumping and recharge rates.

6.4.3.7 *Boundary Element Method*—The boundary element method is a means of reducing a two- or three-dimensional problem to one defined in one or two dimensions **(9)**. In this method the boundary of the problem area is discretized into elements to formulate a boundary integral equation that can be evaluated.

6.4.3.8 *Analytic Element Method*—The analytic element method is a means of using the principle of superposition to combine the solutions to many analytical equations **(10)**. Analytic functions representing stresses, such as wells, line sinks, and circular recharge areas, and features, such as an impermeable barrier, are summed and expressed in terms of discharge potential.

6.4.3.9 Most numerical methods involve replacing the continuous form of the governing differential equation by a finite number of algebraic equations. These algebraic equations are based on subdividing the study area into regular geometric shapes, such as triangles or quadrilaterals or both. The two most common methods of solution are called finite differences and finite elements.

6.4.3.10 *Finite Difference Method*—The most common ground-water flow and transport codes use this method **(11, 12, 13, 14)**. The method requires discretization of the model domain into rectangular cells in two-dimensional models and orthorhombic cells in three-dimensional models. Cells may be arranged to form either a uniform or variably spaced grid. In a model having a uniform grid, all cells have the same length (*l*), width (*w*), and height (*h*). However, the length, width and height may be different, that is, $l_1 = l_2 = l_3$ ..., $w_1 = w_2 = w_3$ ..., $h_1 = h_2 = h_3$ ..., $l_1 \neq w_1 \neq h_1$. In a variably spaced grid, each cell may have length, width, and height, that is, $l_1 \neq l_2 \neq l_3$..., $w_1 \neq w_2 \neq w_3$ ..., $h_1 \neq h_2 \neq h_3$..., $l_1 \neq w_1 \neq h_1$. The finite difference grid may be established as block-centered or mesh-centered.

6.4.3.11 *Block-Centered Grid*—The block-centered formulation places a point, called a node, at the center or the cell, where the hydraulic head or concentration is calculated. Hydraulic and chemical properties are assumed to be uniform over the extent of the cell **(15)**. No-flow boundaries are located at the edge of the cell. Specified-head boundaries are located on the nodes.

6.4.3.12 *Mesh-Centered Grid*—The mesh-centered formulation places a point, also called a node, at the intersection of cell corners. Hydraulic and chemical properties are assumed to be uniform over the area or volume equating to half the distance between nodes. For mesh-centered grids, the no-flow and specified-flow boundaries fall directly on the nodes **(16)**.

6.4.3.13 *Finite Element Method*—Finite elements allow more flexibility in designing a grid. Two-dimensional elements are either triangles or quadrilaterals. Three-dimensional elements are tetrahedrons, hexahedrons, or prisms. Finite elements are better able to approximate irregularly shaped boundaries and to handle internal boundaries such as fault zones **(16)**.

Properties are varied between nodes by a specific function that is usually linear.

7. Model Assumptions

7.1 All mathematical models are based on a set of simplifying assumptions, that affect their use for certain problems. Assumptions can be divided into those associated with the model code, and those associated with problem specific conditions. To avoid applying an otherwise valid model to an inappropriate field situation, knowledge of all of the assumptions that form the basis of the model and consideration of their applicability to the site and problem under evaluations is very important.

8. Types of Errors

8.1 Modeling is subject to errors in both the computer program and in the application of the program to a specific problem. Typographical errors may occur both in coding of the program and in the development of input data sets. These errors can be avoided by thorough quality assurance/quality control procedures. Other errors include truncation, round-off, conceptual, discretization, and data.

8.1.1 *Truncation Error*—The model code usually replaces the governing differential equations with a set of algebraic difference equations that do not yield the exact result. This difference is called the truncation error **(1)**. The level of truncation error in computed results may be estimated by repeating runs or portions of runs with smaller space or time increments, or both. Significant sensitivity of computed results to changes in these increment sizes indicates a significant level of truncation error and the corresponding need for smaller spatial or time increments, or both. Truncation error is not due to the absolute size of grid blocks, but rather to the relative size. For example, if finite difference blocks are more than 1.5 times their neighbor, such error may occur.

8.1.2 *Round-Off Error*—The computer hardware and software used to perform the calculations has a specified accuracy. The difference between the exact result and the computed result is called the round-off error. The accuracy is based on the number of significant digits that are carried in the calculations. Hardware accuracy is controlled by the number of bits used to express a function or a number. Software accuracy is controlled by the specified precision of the numbers. Compared to the other error sources, round-off error is generally negligible **(1)**.

8.1.3 *Conceptual Error*—Improper or incomplete understanding of a ground-water system may result in an incorrect conceptual model. For example, an planar (two-dimensional) model should be applied with care to a three-dimensional problem involving a series of aquifers, hydrologically connected by confining beds, since the model results may not be indicative of the actual field behavior.

8.1.4 *Discretization Error*—Preparation of input data for the model includes gridding the model domain and establishing parameter values for cells, nodes, or elements. Inappropriate gridding, too small or too large, to represent the real system with an input value may result in discretization error. For simplicity or economy, a model domain may be subdivided in to blocks or regions to be assigned equal input parameter values. Inappropriate establishment of regions also may result in discretization error.

8.1.5 *Data Error*—Input data, such as transmissivities, storage coefficients, distribution of head or contaminants, are seldom known accurately or completely. Poor data quality or density may yield incorrect results.

9. Documentation

9.1 *Report*—The purpose of the model report is to communicate findings, to document the procedures and assumptions inherent in the study, and to provide general information for peer review. The report should be a complete document allowing reviewers and decision-makers to formulate their own opinion as to the credibility of the model (see Guide D 5718).

9.2 *Supporting Documentation*—Supporting documentation should be archived such that an independent investigator could duplicate the model results (see Guide D 5718).

10. Keywords

10.1 computer model; ground water; simulation

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