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Standard Guide for
Application of a Ground-Water Flow Model to a Site-Specific Problem[1]

This standard is issued under the fixed designation D5447; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This guide covers the application and subsequent documentation of a ground-water flow model to a particular site or problem. In this context, "ground-water flow model" refers to the application of a mathematical model to the solution of a site-specific ground-water flow problem.

1.2 This guide illustrates the major steps to take in developing a ground-water flow model that reproduces or simulates an aquifer system that has been studied in the field. This guide does not identify particular computer codes, software, or algorithms used in the modeling investigation.

1.3 This guide is specifically written for saturated, isothermal, ground-water flow models. The concepts are applicable to a wide range of models designed to simulate subsurface processes, such as variably saturated flow, flow in fractured media, density-dependent flow, solute transport, and multiphase transport phenomena; however, the details of these other processes are not described in this guide.

1.4 This guide is not intended to be all inclusive. Each ground-water model is unique and may require additional procedures in its development and application. All such additional analyses should be documented, however, in the model report.

1.5 This guide is one of a series of standards on ground-water model applications. Other standards have been prepared on environmental modeling, such as Practice E978.

1.6 *This standard does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to us*

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:*[2]

D653 Terminology Relating to Soil, Rock, and Contained Fluids

E978 Practice for Evaluating Mathematical Models for the Environmental Fate of Chemicals[3]

3. Terminology

3.1 *Definitions:*

3.1.1 *application verification*—using the set of parameter values and boundary conditions from a calibrated model to approximate acceptably a second set of field data measured under similar hydrologic conditions.

3.1.1.1 *Discussion*—Application verification is to be distinguished from code verification, that refers to software testing, comparison with analytical solutions, and comparison with other similar codes to demonstrate that the code represents its mathematical foundation.

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

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

[3] Withdrawn. The last approved version of this historical standard is referenced on www.astm.org.

desired degree of correspondence between the model simulation and observations of the ground-water flow system.

3.1.4 *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.

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

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

3.1.7 *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 deduced with known accuracy.

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

3.1.9 *sensitivity (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.

3.2 For definitions of other terms used in this guide, see Terminology D653.

4. Summary of Guide

4.1 The application of a ground-water flow model ideally would follow several basic steps to achieve an acceptable representation of the physical hydrogeologic system and to document the results of the model study to the end-user, decision-maker, or regulator. These primary steps include the following:

4.1.1 Define study objectives,
4.1.2 Develop a conceptual model,
4.1.3 Select a computer code,
4.1.4 Construct a ground-water flow model,
4.1.5 Calibrate model and perform sensitivity analysis,
4.1.6 Make predictive simulations,
4.1.7 Document modeling study, and
4.1.8 Perform postaudit.

4.2 These steps are designed to ascertain and document an understanding of a system, the transition from conceptual model to mathematical model, and the degree of uncertainty in the model predictions. The steps presented in this guide should generally be followed in the order they appear in the guide; however, there is often significant iteration between steps. All steps outlined in this guide are required for a model that simulates measured field conditions. In cases where the model is only used to understand a problem conceptually, not all steps are necessary. For example, if no site-specific data are available, the calibration step would be omitted.

5. Significance and Use

5.1 According to the National Research Council (**1**),[4] model applications are useful tools to:

5.1.1 Assist in problem evaluation,
5.1.2 Design remedial measures,
5.1.3 Conceptualize and study ground-water flow processes,
5.1.4 Provide additional information for decision making, and
5.1.5 Recognize limitations in data and guide collection of new data.

5.2 Ground-water models are routinely employed in making environmental resource management decisions. The model supporting these decisions must be scientifically defensible and decision-makers must be informed of the degree of uncertainty in the model predictions. This has prompted some state agencies to develop standards for ground-water modeling (**2**). This guide provides a consistent framework within which to develop, apply, and document a ground-water flow model.

5.3 This guide presents steps ideally followed whenever a ground-water flow model is applied. The ground-water flow model will be based upon a mathematical model that may use numerical, analytical, or any other appropriate technique.

5.4 This guide should be used by practicing ground-water modelers and by those wishing to provide consistency in modeling efforts performed under their direction.

5.5 Use of this guide to develop and document a ground-water flow model does not guarantee that the model is valid. This guide simply outlines the necessary steps to follow in the modeling process. For example, development of an equivalent porous media model in karst terrain may not be valid if significant ground-water flow takes place in fractures and solution channels. In this case, the modeler could follow all steps in this guide and not end up with a defensible model.

6. Procedure

6.1 The procedure for applying a ground-water model includes the following steps: define study objectives, develop a conceptual model, select a computer code or algorithm, construct a ground-water flow model, calibrate the model and perform sensitivity analysis, make predictive simulations, document the modeling process, and perform a postaudit. These steps are generally followed in order, however, there is substantial overlap between steps, and previous steps are often revisited as new concepts are explored or as new data are obtained. The iterative modeling approach may also require the reconceptualization of the problem. An example of these feedback loops is shown in Fig. 1. These basic modeling steps are discussed below.

6.2 Definition of the study objectives is an important step in applying a ground-water flow model. The objectives aid in determining the level of detail and accuracy required in the model simulation. Complete and detailed objectives would ideally be specified prior to any modeling activities.

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[4] The boldface numbers in parentheses refer to the list of references at the end of this standard.

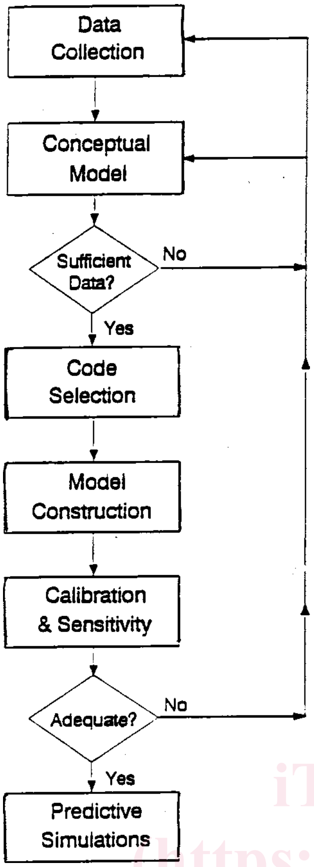

FIG. 1 Flow Chart of the Modeling Process

6.3 A conceptual model of a ground-water flow and hydrologic system is an interpretation or working description of the characteristics and dynamics of the physical hydrogeologic system. The purpose of the conceptual model is to consolidate site and regional hydrogeologic and hydrologic data into a set of assumptions and concepts that can be evaluated quantitatively. Development of the conceptual model requires the collection and analysis of hydrogeologic and hydrologic data pertinent to the aquifer system under investigation. Standard guides and practices exist that describe methods for obtaining hydrogeologic and hydrologic data.

6.3.1 The conceptual model identifies and describes important aspects of the physical hydrogeologic system, including: geologic and hydrologic framework, media type (for example, fractured or porous), physical and chemical processes, hydraulic properties, and sources and sinks (water budget). These components of the conceptual model may be described either in a separate document or as a chapter within the model report. Include illustrations, where appropriate, to support the narrative, for example, contour maps, cross sections, or block diagrams, or combination thereof. Each aspect of the conceptual model is described as follows:

6.3.1.1 Geologic framework is the distribution and configuraton of aquifer and confining units. Of primary interest are the thickness, continuity, lithology, and geologic structure of those units that are relevant to the purpose of the study. The aquifer system domain, that may be composed of interconnected aquifers and confining units, often extends beyond the domain of interest. In this case, describe the aquifer system in detail within the domain of interest and at least in general elsewhere. Analysis of the geologic framework results in listings, tabulations, or maps, or combination thereof, of the thickness, extent, and properties of each relevant aquifer and confining unit.

6.3.1.2 Hydrologic framework in the conceptual model includes the physical extents of the aquifer system, hydrologic features that impact or control the ground-water flow system, analysis of ground-water flow directions, and media type. The conceptual model must address the degree to which the aquifer system behaves as a porous media. If the aquifer system is significantly fractured or solutioned, the conceptual model must address these issues. Hydrologic framework also includes flow system boundaries that may not be physical and can change with time, such as ground-water divides. Fluid potential (head) measurements allow assessment of the rate and direction of ground-water flow. In addition, the mathematical model is typically calibrated against these values (see 6.5). Water level measurements within the ground-water system are tabulated, both spatially and temporally. This analysis of the flow system includes the assessment of vertical and horizontal gradients, delineation of ground-water divides, and mapping of flow lines.

6.3.1.3 Hydraulic properties include the transmissive and storage characteristics of the aquifer system. Specific examples of hydraulic properties include transmissivity, hydraulic conductivity, storativity, and specific yield. Hydraulic properties may be homogeneous or heterogeneous throughout the model domain. Certain properties, such as hydraulic conductivity, may also have directionality, that is, the property may be anisotropic. It is important to document field and laboratory measurements of these properties in the conceptual model to set bounds or acceptable ranges for guiding the model calibration.

6.3.1.4 Sources and sinks of water to the aquifer system impact the pattern of ground-water flow. The most common examples of sources and sinks include pumping or injection wells, infiltration, evapotranspiration, drains, leakage across confining layers and flow to or from surface water bodies. Identify and describe sources and sinks within the aquifer system in the conceptual model. The description includes the rates and the temporal variability of the sources and sinks. A water budget should be developed as part of the conceptual model.

6.3.2 Provide an analysis of data deficiencies and potential sources of error with the conceptual model. The conceptual model usually contains areas of uncertainty due to the lack of field data. Identify these areas and their significance to the conceptual model evaluated with respect to project objectives. In cases where the system may be conceptualized in more than one way, these alternative conceptual models should be described and evaluated.

6.4 Computer code selection is the process of choosing the appropriate software algorithm, or other analysis technique, capable of simulating the characteristics of the physical hydrogeologic system, as identified in the conceptual model. The computer code must also be tested for the intended use and be well documented (**3-5**).

6.4.1 Other factors may also be considered in the decision-making process, such as model analyst's experience and those described below for model construction. Important aspects of the model construction process, such as dimensionality, will determine the capabilities of the computer code required for the model. Provide a narrative in the modeling report justifying the computer code selected for the model study.

6.5 Ground-water flow model construction is the process of transforming the conceptual model into a mathematical form. The ground-water flow model typically consists of two parts, the data set and the computer code. The model construction process includes building the data set utilized by the computer code. Fundamental components of the ground-water flow model include: dimensionality, discretization, boundary and initial conditions, and hydraulic properties.

6.5.1 Spatial dimensionality is determined both by the objectives of the investigation and by the nature of the ground-water flow system. For example, conceptual modeling studies may use simple one-dimensional solutions in order to test alternate conceptualizations. Two-dimensional modeling may be warranted if vertical gradients are negligible. If vertical gradients are significant or if there are several aquifers in the flow system, a two-dimensional cross section or (quasi-)three-dimensional model may be appropriate. A quasi-three-dimensional approach is one in which aquitards are not explicitly discretized but are approximated using a leakage term (**6**).

6.5.2 Temporal dimensionality is the choice between steady-state or transient flow conditions. Steady-state simulations produce average or long-term results and require that a true equilibrium case is physically possible. Transient analyses are typically performed when boundary conditions are varied through time or when study objectives require answers at more than one point in time.

6.5.3 In numerical models, spatial discretization is a critical step in the model construction process (**6**). In general, finer discretization produces a more accurate solution to the governing equations. There are practical limits to the number of nodes, however. In order to achieve acceptable results with the minimum number of nodes, the model grid may require finer discretization in areas of interest or where there are large spatial changes in aquifer parameters or hydraulic gradient. In designing a numerical model, it is advisable to locate nodes as close as possible to pumping wells, to locate model edges and hydrologic boundaries accurately, and to avoid large contrasts in adjacent nodal spacings (**7**).

6.5.4 Temporal discretization is the selection of the number and size of time steps for the period of transient numerical model simulations. Choose time steps or intervals to minimize errors caused by abrupt changes in boundary conditions. Generally, small time steps are used in the vicinity of such changes to improve accuracy (**8**). Some numerical time-stepping schemes place additional constraints on the maximum time-step size due to numerical stability.

6.5.5 Specifying the boundary conditions of the ground-water flow model means assigning a boundary type to every point along the three-dimensional boundary surface of the aquifer system and to internal sources and sinks (**9**). Boundary conditions fall into one of five categories: specified head or Dirichlet, specified flux or Neumann, and mixed or Cauchy boundary conditions, free surface boundary, and seepage face. It is desirable to include only natural hydrologic boundaries as boundary conditions in the model. Most numerical models, however, employ a grid that must end somewhere. Thus, it is often unavoidable to specify artificial boundaries at the edges of the model. When these grid boundaries are sufficiently remote from the area of interest, the artificial conditions on the grid boundary do not significantly impact the predictive capabilities of the model. However, the impact of artificial boundaries should always be tested and thoroughly documented in the model report.

6.5.6 Initial conditions provide a starting point for transient model calculations. In numerical ground-water flow models, initial conditions consist of hydraulic heads specified for each model node at the beginning of the simulation. Initial conditions may represent a steady-state solution obtained from the same model. Accurately specify initial conditions for transient models. Steady-state models do not require initial conditions.

6.5.7 In numerical modeling, each node or element is assigned a value for each hydraulic property required by the ground-water flow model. Other types of models, such as many analytical models, specify homogeneous property values. The most common hydraulic properties are horizontal and vertical hydraulic conductivity (or transmissivity) and storage coefficients. Hydraulic property values are assigned in the model based upon geologic and aquifer testing data. Generally, hydraulic property values are assigned in broad zones having similar geologic characteristics (**10**). Geostatistical techniques, such as kriging, are also commonly used to assign property values at model nodes when sufficient data are available.

6.6 Calibration of the ground-water flow model is the process of adjusting hydraulic parameters, boundary conditions, and initial conditions within reasonable ranges to obtain a match between observed and simulated potentials, flow rates, or other calibration targets. The range over which model parameters and boundary conditions may be varied is determined by data presented in the conceptual model. In the case where parameters are well characterized by field measurements, the range over which that parameter is varied in the model should be consistent with the range observed in the field. The degree of fit between model simulations and field measurements can be quantified using statistical techniques (**2**).

6.6.1 In practice, model calibration is frequently accomplished through trial-and-error adjustment of the model's input data to match field observations (**10**). Automatic inverse techniques are another type of calibration procedure (**11-13**). The calibration process continues until the degree of correspondence between the simulation and the physical hydrogeologic system is consistent with the objectives of the project.

6.6.2 The calibration is evaluated through analysis of residuals. A residual is the difference between the observed and simulated variable. Calibration may be viewed as a regression analysis designed to bring the mean of the residuals close to zero and to minimize the standard deviation of the residuals (**10**). Statistical tests and illustrations showing the distribution of residuals are presented to document the calibration. Ideally,