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Designation: D 5447 – 93$^{\epsilon1}$

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

This standard is issued under the fixed designation D 5447; 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.

ϵ^1 Note—Paragraph 1.7 was added editorially October 1998.

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 E 978.

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:*

D 653 Terminology Relating to Soil, Rock, and Contained Fluids[2]

E 978 Practice for Evaluating Environmental Fate Models 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 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.

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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 11.04.

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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 D 653.

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.

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

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

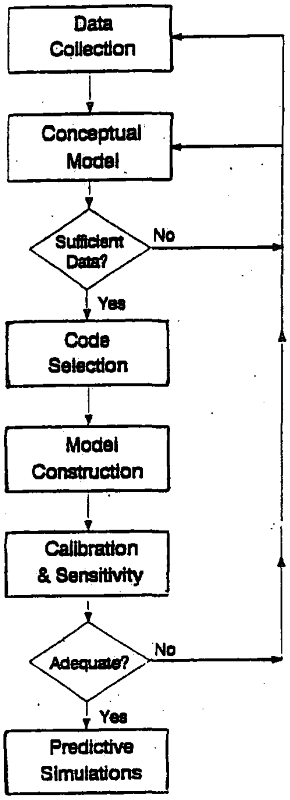

FIG. 1 Flow Chart of the Modeling Process

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, criteria for an acceptable calibration should be established prior to starting the calibration.

6.6.3 Calibration often necessitates reconstruction of portions of the model, resulting in changes or refinements in the conceptual model. Both possibilities introduce iteration into the modeling process whereby the modeler revisits previous steps to achieve a better representation of the physical system.

6.6.4 In both trial-and-error and inverse techniques, sensitivity analysis plays a key role in the calibration process by identifying those parameters that are most important to model reliability. Sensitivity analysis is used extensively in inverse techniques to make adjustments in model parameter values.

6.6.5 Calibration of a ground-water flow model to a single set of field measurements does not guarantee a unique solution. In order to reduce the problem of nonuniqueness, the model calculations may be compared to another set of field observations that represent a different set of boundary conditions or stresses. This process is referred to in the ground-water modeling literature as either validation (**1**) or verification (**14, 15**). The term verification is adopted in this guide. In model verification, the calibrated model is used to simulate a different set of aquifer stresses for which field measurements have been made. The model results are then compared to the field measurements to assess the degree of correspondence. If the comparison is not favorable, additional calibration or data collection is required. Successful verification of the ground-water flow model results in a higher degree of confidence in model predictions. A calibrated but unverified model may still be used to perform predictive simulations when coupled with a careful sensitivity analysis (**15**).

6.7 Sensitivity analysis is a quantitative method of determining the effect of parameter variation on model results. The purpose of a sensitivity analysis is to quantify the uncertainty in the calibrated model caused by uncertainty in the estimates of aquifer parameters, stresses, and boundary conditions (**6**). It is a means to identify the model inputs that have the most influence on model calibration and predictions (**1**). Perform sensitivity analysis to provide users with an understanding of the level of confidence in model results and to identify data deficiencies (**16**).

6.7.1 Sensitivity analysis is performed during model calibration and during predictive analyses. Model sensitivity provides a means of determining the key parameters and boundary conditions to be adjusted during model calibration. Sensitivity analysis is used in conjunction with predictive simulations to assess the effect of parameter uncertainty on model results.

6.7.2 Sensitivity of a model parameter is often expressed as the relative rate of change of a selected model calculation with respect to that parameter (**17**). If a small change in the input parameter or boundary condition causes a significant change in the output, the model is sensitive to that parameter or boundary condition.

6.8 Application of the ground-water flow model to a particular site or problem often includes predictive simulations. Predictive simulations are the analyses of scenarios defined as part of the study objectives. Document predictive simulations with appropriate illustrations as necessary in the model report.

6.8.1 Boundary conditions are often selected during model construction based upon existing or past ground-water flow conditions. Boundary conditions used in the calibrated model may not be appropriate for all predictive simulations (**18**). If the model simulations result in unusually large hydrologic stresses or if new stresses are placed in proximity to model boundaries, evaluate the sensitivity of the predictions to the boundary conditions. This may produce additional iteration in the modeling process.

6.9 In cases where the ground-water flow model has been used for predictive purposes, a postaudit may be performed to determine the accuracy of the predictions. While model calibration and verification demonstrate that the model accurately simulate past behavior of the system, the postaudit tests whether the model can predict future system behavior (**15**). Postaudits are normally performed several years after submittal of the modeling report and are therefore documented in a separate report.

7. Report

7.1 The purpose of the model report is to communicate findings, to document the procedures and assumptions inherent in the study, and to provide detailed 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. The report should be detailed enough that an independent modeler could duplicate the model results. The model report should describe all aspects of the modeling study outlined in this guide. An example table of contents for a modeling report is presented in Appendix X1.

8. Keywords

8.1 computer model; ground-water; simulation

APPENDIX

(Nonmandatory Information)

X1. GROUND-WATER FLOW MODEL REPORT

X1.1 See Fig. X1.1.

1.0 Introduction
- 1.1 General Setting
- 1.2 Study Objectives

2.0 Conceptual Model
- 2.1 Aquifer System Framework
- 2.2 Ground-Water Flow System
- 2.3 Hydrologic Boundaries
- 2.4 Hydraulic Properties
- 2.5 Sources and Sinks
- 2.6 Water Budget

3.0 Computer Code
- 3.1 Code Selection
- 3.2 Code Description

4.0 Ground-Water Flow Model Construction
- 4.1 Model Grid
- 4.2 Hydraulic Parameters
- 4.3 Boundary Conditions
- 4.4 Selection of Calibration Targets

5.0 Calibration
- 5.1 Residual Analysis
- 5.2 Sensitivity Analysis
- 5.3 Model Verification

6.0 Predictive Simulations

7.0 Summary and Conclusions
- 7.1 Model Assumptions and Limitations
- 7.2 Model Predictions
- 7.3 Recommendations

8.0 References

Appendices: Model Input Files

FIG. X1.1 Example Table of Contents of Ground-Water Flow Model Report

REFERENCES

(1) National Research Council, *Ground Water Models: Scientific and Regulatory Applications*, National Academy Press, Washington, DC, 1990.

(2) *Scientific and Technical Standards for Hazardous Waste Sites, Volume 2: Exposure Assessment, Chapter 4*, "Standards for Mathematical Modeling of Ground Water Flow and Contaminant Transport at Hazardous Waste Sites," State of California, Toxic Substances Control Program, DRAFT Standards, August 1990.

(3) van der Heijde, P. K. M., *Quality Assurance in Computer Simulations of Ground Water Contamination*, EPA/600/J-87/084, PB-0124524, 1987.

(4) U.S. Environmental Protection Agency, *Selection Criteria for Mathematical Models Used in Exposure Assessments: Ground-Water Models*, EPA/600/8-88/075, 1987.

(5) Silling, S. A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission, NUREG-0856, 1983.

(6) Anderson, M. P., and Woessner, W. W., *Applied Groundwater Modeling: Simulation of Flow and Advective Transport*, Academic Press, Inc., New York, NY, 1992.

(7) Trescott, P. C., Pinder, G. F., and Larson, S. P., "Finite-Difference Model for Aquifer Simulation in Two Dimensions with Results of Numerical Experiments," *U.S. Geological Survey TWRI*, Book 7, Chapter C1, 1976.

(8) Mercer, J. W., and Faust, C. R., *Ground-Water Modeling: Numerical Models, Ground Water*, Vol 18, No. 4, 1980, pp. 395–409.

(9) Franke, O. L., Reilly, T. E., and Bennett, G. D., "Definition of Boundary and Initial Conditions in the Analysis of Saturated Ground-Water Flow Systems—An Introduction," *U.S. Geological Survey, Techniques of Water Resources Investigations*, Book 3, Chapter B5, Vol 15, 1987.

(10) Konikow, I. F., "Calibration of Ground-Water Models," *Proceedings of the Specialty Conference on Verification of Mathematical and Physical Models in Hydraulic Engineering*, ASCE, College Park, MD, Aug. 9–11, 1978, pp. 87–93.

(11) Cooley, R. L., *A Method of Estimating Parameters and Assessing Reliability for Models of Steady State Ground-Water Flow. I. Theory and Numerical Properties*, WRR, Vol 13, No. 2, 1977, pp. 318–324.

(12) Faust, C. R., and Mercer, J. W., "Ground-Water Modeling: Recent Developments," *Ground Water*, Vol 18, No. 6, 1980, pp. 569–577.

(13) Yeh, W. W-G., "Review of Parameter Identification Procedures in Groundwater Hydrology: The Inverse Problem," *WRR*, Vol 22, 1986, pp. 95–108.

(14) Wang, H. F., and Anderson, M. P., *Introduction to Groundwater Modeling: Finite Difference and Finite Element Methods*, W. H. Freeman and Co., San Francisco, CA, 1982.

(15) Anderson, M. P., and Woessner, W. W., "The Role of the Postaudit in Model Validation," submitted to *Advances in Water Resources, Special Issue on Model Validation*, January 1992, 9.

(16) U.S. Environmental Protection Agency, *Resolution on the Use of Mathematical Models by EPA for Regulatory Assessment and Decision-Making*, EPA-SAB-EEC-89-012, 1989.

(17) van der Heijde, P. K. M., *Quality Assurance and Quality Control in Groundwater Modeling*, International Ground Water Modeling Center, GWMI 89-04, 1989.

(18) Franke, O. L., and Reilly, T. E., "*The Effects of Boundary Conditions on the Steady-State Response of Three Hypothetical Ground-Water Systems—Results and Implications of Numerical Experiments*," *U.S. Geological Survey Water Supply Paper 2315*, 1987.

Designation: D 5490 – 93$^{\epsilon 1}$

Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information[1]

This standard is issued under the fixed designation D 5490; 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.

ε¹ Note—Paragraph 1.9 was added editorially October 1998.

1. Scope

1.1 This guide covers techniques that should be used to compare the results of ground-water flow model simulations to measured field data as a part of the process of calibrating a ground-water model. This comparison produces quantitative and qualitative measures of the degree of correspondence between the simulation and site-specific information related to the physical hydrogeologic system.

1.2 During the process of calibration of a ground-water flow model, each simulation is compared to site-specific information such as measured water levels or flow rates. The degree of correspondence between the simulation and the physical hydrogeologic system can then be compared to that for previous simulations to ascertain the success of previous calibration efforts and to identify potentially beneficial directions for further calibration efforts.

1.3 By necessity, all knowledge of a site is derived from observations. This guide does not address the adequacy of any set of observations for characterizing a site.

1.4 This guide does not establish criteria for successful calibration, nor does it describe techniques for establishing such criteria, nor does it describe techniques for achieving successful calibration.

1.5 This guide is written for comparing the results of numerical ground-water flow models with observed site-specific information. However, these techniques could be applied to other types of ground-water related models, such as analytical models, multiphase flow models, noncontinuum (karst or fracture flow) models, or mass transport models.

1.6 This guide is one of a series of guides on ground-water modeling codes (software) and their applications. Other standards have been prepared on environmental modeling, such as Practice E 978.

1.7 The values stated in SI units are to be regarded as the standard.

1.8 *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 use.*

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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 11.04.

3.1.3 *censored data*—knowledge that the value of a variable in the physical hydrogeologic system is less than or greater than a certain value, without knowing the exact value.

3.1.3.1 *Discussion*—For example, if a well is dry, then the potentiometric head at that place and time must be less than the elevation of the screened interval of the well although its specific value is unknown.

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

3.1.5 *ground-water flow model*—an application of a mathematical model to represent a ground-water flow system.

3.1.6 *hydrologic condition*—a set of ground-water inflows or outflows, boundary conditions, and hydraulic properties that cause potentiometric heads to adopt a distinct pattern.

3.1.7 *residual*—the difference between the computed and observed values of a variable at a specific time and location.

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

3.1.8.1 *Discussion*—For the purposes of this guide, a simulation refers to an individual modeling run. However, simulation is sometimes also used broadly to refer to the process of modeling in general.

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

4. Summary of Guide

4.1 Quantitative and qualitative comparisons are both essential. Both should be used to evaluate the degree of correspondence between a ground-water flow model simulation and site-specific information.

4.2 Quantitative techniques for comparing a simulation with site-specific information include:

4.2.1 Calculation of residuals between simulated and measured potentiometric heads and calculation of statistics regarding the residuals. Censored data resulting from detection of dry or flowing observation wells, reflecting information that the head is less than or greater than a certain value without knowing the exact value, should also be used.

4.2.2 Detection of correlations among residuals. Spatial and temporal correlations among residuals should be investigated. Correlations between residuals and potentiometric heads can be detected using a scattergram.

4.2.3 Calculation of flow-related residuals. Model results should be compared to flow data, such as water budgets, surface water flow rates, flowing well discharges, vertical gradients, and contaminant plume trajectories.

4.3 Qualitative considerations for comparing a simulation with site-specific information include:

4.3.1 Comparison of general flow features. Simulations should reproduce qualitative features in the pattern of ground-water contours, including ground-water flow directions, mounds or depressions (closed contours), or indications of surface water discharge or recharge (cusps in the contours).

4.3.2 Assessment of the number of distinct hydrologic conditions to which the model has been successfully calibrated. It is usually better to calibrate to multiple scenarios, if the scenarios are truly distinct.

4.3.3 Assessment of the reasonableness or justifiability of the input aquifer hydrologic properties given the aquifer materials which are being modeled. Modeled aquifer hydrologic properties should fall within realistic ranges for the physical hydrogeologic system, as defined during conceptual model development.

5. Significance and Use

5.1 During the process of calibration of a ground-water flow model, each simulation is compared to site-specific information to ascertain the success of previous calibration efforts and to identify potentially beneficial directions for further calibration efforts. Procedures described herein provide guidance for making comparisons between ground-water flow model simulations and measured field data.

5.2 This guide is not meant to be an inflexible description of techniques comparing simulations with measured data; other techniques may be applied as appropriate and, after due consideration, some of the techniques herein may be omitted, altered, or enhanced.

6. Quantitative Techniques

6.1 Quantitative techniques for comparing simulations to site-specific information include calculating potentiometric head residuals, assessing correlation among head residuals, and calculating flow residuals.

6.1.1 *Potentiometric Head Residuals*—Calculate the residuals (differences) between the computed heads and the measured heads:

$$r_i = h_i - H_i \tag{1}$$

where:

r_i = the residual,
H_i = the measured head at point i,
h_i = the computed head at the approximate location where H_i was measured.

If the residual is positive, then the computed head was too high; if negative, the computed head was too low. Residuals cannot be calculated from censored data.

NOTE 1—For drawdown models, residuals can be calculated from computed and measured drawdowns rather than heads.

NOTE 2—Comparisons should be made between point potentiometric heads rather than ground-water contours, because contours are the result of interpretation of data points and are not considered basic data in and of themselves.[4] Instead, the ground-water contours are considered to reflect features of the conceptual model of the site. The ground-water flow model should be true to the essential features of the conceptual model and not to their representation.

NOTE 3—It is desirable to set up the model so that it calculates heads at the times and locations where they were measured, but this is not always possible or practical. In cases where the location of a monitoring well does not correspond exactly to one of the nodes where heads are computed in the simulation, the residual may be adjusted (for example, computed heads may be interpolated, extrapolated, scaled, or otherwise transformed) for use in calculating statistics. Adjustments may also be necessary when the times of measurements do not correspond exactly with the times when heads are calculated in transient simulations; when many observed heads

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[4] Cooley, R. L., and Naff, R. L., "Regression Modeling of Ground-Water Flow," *USGS Techniques of Water Resources Investigations*, Book 3, Chapter B4, 1990.

are clustered near a single node; where the hydraulic gradient changes significantly from node to node; or when observed head data is affected by tidal fluctuations or proximity to a specified head boundary.

6.1.2 *Residual Statistics*—Calculate the maximum and minimum residuals, a residual mean, and a second-order statistic, as described in the following sections.

6.1.2.1 *Maximum and Minimum Residuals*—The maximum residual is the residual that is closest to positive infinity. The minimum residual is the residual closest to negative infinity. Of two simulations, the one with the maximum and minimum residuals closest to zero has a better degree of correspondence, with regard to this criterion.

NOTE 4—When multiple hydrologic conditions are being modeled as separate steady-state simulations, the maximum and minimum residual can be calculated for the residuals in each, or for all residuals in all scenarios, as appropriate. This note also applies to the residual mean (see 6.1.2.2) and second-order statistics of the residuals (see 6.1.2.4).

6.1.2.2 *Residual Mean*—Calculate the residual mean as the arithmetic mean of the residuals computed from a given simulation:

$$R = \frac{\sum_{i=1}^{n} r_i}{n} \quad (2)$$

where:

R = the residual mean and

n = the number of residuals.

Of two simulations, the one with the residual mean closest to zero has a better degree of correspondence, with regard to this criterion (assuming there is no correlation among residuals).

6.1.2.3 If desired, the individual residuals can be weighted to account for differing degrees of confidence in the measured heads. In this case, the residual mean becomes the weighted residual mean:

$$R = \frac{\sum_{i=1}^{n} w_i r_i}{n \sum_{i=1}^{n} w_i} \quad (3)$$

where w_i is the weighting factor for the residual at point i. The weighting factors can be based on the modeler's judgment or statistical measures of the variability in the water level measurements. A higher weighting factor should be used for a measurement with a high degree of confidence than for one with a low degree of confidence.

NOTE 5—It is possible that large positive and negative residuals could cancel, resulting in a small residual mean. For this reason, the residual mean should never be considered alone, but rather always in conjunction with the other quantitative and qualitative comparisons.

6.1.2.4 *Second-Order Statistics*—Second-order statistics give measures of the amount of spread of the residuals about the residual mean. The most common second-order statistic is the standard deviation of residuals:

$$s = \left\{ \frac{\sum_{i=1}^{n} (r_i - R)^2}{(n-1)} \right\}^{\frac{1}{2}} \quad (4)$$

where s is the standard deviation of residuals. Smaller values of the standard deviation indicate better degrees of correspondence than larger values.

6.1.2.5 If weighting is used, calculate the weighted standard deviation:

$$s = \left\{ \frac{\sum_{i=1}^{n} w_i (r_i - R)^2}{(n-1) \sum_{i=1}^{n} w_i} \right\}^{\frac{1}{2}} \quad (5)$$

NOTE 6—Other norms of the residuals are less common but may be revealing in certain cases.[5,6] For example, the mean of the absolute values of the residuals can give information similar to that of the standard deviation of residuals.

NOTE 7—In calculating the standard deviation of residuals, advanced statistical techniques incorporating information from censored data could be used. However, the effort would usually not be justified because the standard deviation of residuals is only one of many indicators involved in comparing a simulation with measured data, and such a refinement in one indicator is unlikely to alter the overall assessment of the degree of correspondence.

6.1.3 *Correlation Among Residuals*—Spatial or temporal correlation among residuals can indicate systematic trends or bias in the model. Correlations among residuals can be identified through listings, scattergrams, and spatial or temporal plots. Of two simulations, the one with less correlation among residuals has a better degree of correspondence, with regard to this criterion.

6.1.3.1 *Listings*—List residuals by well or piezometer, including the measured and computed values to detect spatial or temporal trends. Figures X1.1 and X1.2 present example listings of residuals.

6.1.3.2 *Scattergram*—Use a scattergram of computed versus measured heads to detect trends in deviations. The scattergram is produced with measured heads on the abscissa (horizontal axis) and computed heads on the ordinate (vertical axis). One point is plotted on this graph for each pair. If the points line up along a line with zero intercept and 45° angle, then there has been a perfect match. Usually, there will be some scatter about this line, hence the name of the plot. A simulation with a small degree of scatter about this line has a better correspondence with the physical hydrogeologic system than a simulation with a large degree of scatter. In addition, plotted points in any area of the scattergram should not all be grouped above or below the line. Figures X1.3 and X1.4 show sample scattergrams.

6.1.3.3 *Spatial Correlation*—Plot residuals in plan or section to identify spatial trends in residuals. In this plot, the residuals, including their sign, are plotted on a site map or cross section. If possible or appropriate, the residuals can also be contoured. Apparent trends or spatial correlations in the residuals may indicate a need to refine aquifer parameters or boundary conditions, or even to reevaluate the conceptual model (for example, add spatial dimensions or physical processes). For example, if all of the residuals in the vicinity of a no-flow boundary are positive, then the recharge may need to

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[5] Ghassemi, F., Jakeman, A. J., and Thomas, G. A., "Ground-Water Modeling for Salinity Management: An Australian Case Study," *Ground Water*, Vol 27, No. 3, 1989, pp. 384–392.

[6] Konikow, L. F., *Calibration of Ground-Water Models, Proceedings of the Specialty Conference on Verification of Mathematical and Physical Models in Hydraulic Engineering*, ASCE, College Park, MD, Aug. 9–11, 1978, pp. 87–93.

be reduced or the hydraulic conductivity increased. Figure X1.5 presents an example of a contour plot of residuals in plan view. Figure X1.6 presents an example of a plot of residuals in cross section.

6.1.3.4 *Temporal Correlation*—For transient simulations, plot residuals at a single point versus time to identify temporal trends. Temporal correlations in residuals can indicate the need to refine input aquifer storage properties or initial conditions. Figure X1.7 presents a typical plot of residuals versus time.

6.1.4 *Flow-Related Residuals*—Often, information relating to ground-water velocities is available for a site. Examples include water budgets, surface water flow rates, flowing well discharges, vertical gradients, and contaminant plume trajectories (ground-water flow paths). All such quantities are dependent on the hydraulic gradient (the spatial derivative of the potentiometric head). Therefore, they relate to the overall structure of the pattern of potentiometric heads and provide information not available from point head measurements. For each such datum available, calculate the residual between its computed and measured values. If possible and appropriate, calculate statistics on these residuals and assess their correlations, in the manner described in 5.1 and 5.2 for potentiometric head residuals.

6.1.4.1 *Water Budgets and Mass Balance*—For elements of the water budget for a site which are calculated (as opposed to specified in the model input) (for example, base flow to a stream), compare the computed and the measured (or estimated) values. In addition, check the computed mass balance for the simulation by comparing the sum of all inflows to the sum of all outflows and changes in storage. Differences of more than a few percent in the mass balance indicate possible numerical problems and may invalidate simulation results.

6.1.4.2 *Vertical Gradients*—In some models, it may be more important to accurately represent the difference in heads above and below a confining layer, rather than to reproduce the heads themselves. In such a case, it may be acceptable to tolerate a correlation between the head residuals above and below the layer if the residual in the vertical gradient is minimized.

6.1.4.3 *Ground-Water Flow Paths*—In some models, it may be more important to reproduce the pattern of streamlines in the ground-water flow system rather than to reproduce the heads themselves (for example, when a flow model is to be used for input of velocities into a contaminant transport model). In this case, as with the case of vertical gradients in 6.1.4.2 it may be acceptable to tolerate some correlation in head residuals if the ground-water velocity (magnitude and direction) residuals are minimized.

7. Qualitative Considerations

7.1 *General Flow Features*—One criterion for evaluating the degree of correspondence between a ground-water flow model simulation and the physical hydrogeologic system is whether or not essential qualitative features of the potentiometric surface are reflected in the model. The overall pattern of flow directions and temporal variations in the model should correspond with those at the site. For example:

7.1.1 If there is a mound or depression in the potentiometric surface at the site, then the modeled contours should also indicate a mound or depression in approximately the same area.

7.1.2 If measured heads indicate or imply cusps in the ground-water contours at a stream, then these features should also appear in contours of modeled heads.

7.2 *Hydrologic Conditions*—Identify the different hydrologic conditions that are represented by the available data sets. Choose one data set from each hydrologic condition to use for calibration. Use the remaining sets for verification.

7.2.1 *Uniqueness (Distinct Hydrologic Conditions)*—The number of distinct hydrologic conditions that a given set of input aquifer hydrologic properties is capable of representing is an important qualitative measure of the performance of a model. It is usually better to calibrate to multiple conditions, if the conditions are truly distinct. Different hydrologic conditions include, but are not limited to, high and low recharge; conditions before and after pumping or installation of a cutoff wall or cap; and high and low tides, flood stages for adjoining surface waters, or installation of drains. By matching different hydrologic conditions, the uniqueness problem is addressed, because one set of heads can be matched with the proper ratio of ground-water flow rates to hydraulic conductivities; whereas, when the flow rates are changed, representing a different condition, the range of acceptable hydraulic conductivities becomes much more limited.

7.2.2 *Verification (Similar Hydrologic Conditions)*—When piezometric head data are available for two times of similar hydrologic conditions, only one of those conditions should be included in the calibration data sets because they are not distinct. However, the other data set can be used for model verification. In the verification process, the modeled piezometric heads representing the hydrologic condition in question are compared, not to the calibration data set, but to the verification data set. The resulting degree of correspondence can be taken as an indicator or heuristic measure of the ability of the model to represent new hydrologic conditions within the range of those to which the model was calibrated.

NOTE 8—When only one data set is available, it is inadvisable to artificially split it into separate "calibration" and "verification" data sets. It is usually more important to calibrate to piezometric head data spanning as much of the modeled domain as possible.

NOTE 9—Some researchers maintain that the word "verification" implies a higher degree of confidence than is warranted.[7] Used here, the verification process only provides a method for estimating confidence intervals on model predictions.

7.3 *Input Aquifer Hydraulic Properties*—A good correspondence between a ground-water flow model simulation and site-specific information, in terms of quantitative measures, may sometimes be achieved using unrealistic aquifer hydraulic properties. This is one reason why emphasis is placed on the ability to reproduce multiple distinct hydrologic stress scenarios. Thus, a qualitative check on the degree of correspondence between a simulation and the physical hydrogeologic system should include an assessment of the likely ranges of hydraulic properties for the physical hydrogeologic system at

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[7] Konikow, L. F., and Bredehoeft, J. D., "Ground-Water Models Cannot Be Validated," *Adv. Wat. Res.* Vol 15, 1992, pp. 75–83.

the scale of the model or model cells and whether the properties used in the model lie within those ranges.

8. Report

8.1 When a report for a ground-water flow model application is produced, it should include a description of the above comparison tests which were performed, the rationale for selecting or omitting comparison tests, and the results of those comparison tests.

9. Keywords

9.1 calibration; computer; ground water; modeling

APPENDIX

(Nonmandatory Information)

X1. EXAMPLES

X1.1 Fig. X1.1 and Fig. X1.2 present sample listings of residuals, as described in 6.1.3.1. These listings tabulate the residuals for simulations of two hydrologic conditions with the same model. Note that some of the wells do not have measurements for both simulations. Simulated heads for these wells are still reported as an aid to detecting temporal trends in the heads for different aquifer stresses. Some censored water level data were available for this site. For these data, the table merely indicates whether or not the simulation is consistent with the censored data.

X1.2 Fig. X1.3 and Fig. X1.4 show sample scattergrams, as described in 6.1.3.2. The scattergram on Fig. X1.3 indicates a good match between modeled and measured potentiometric heads because there is little or no pattern between positive and negative residuals and because the magnitude of the residuals is small compared to the total change in potentiometric head across the site. The residuals shown on the scattergram on Fig. X1.4 have the same maximum, minimum, mean, and standard deviation as those shown on Fig. X1.3, but show a pattern of positiveresiduals upgradient and negative residuals downgradient. However, even though the statistical comparisons would indicate a good degree of correspondence, this model may overestimate seepage velocities because the simulated hydraulic gradient is higher than the measured hydraulic gradient. Therefore this model may need to be improved if the heads are to be input into a mass transport model.

Example Site
Stress scenario #1
Simulation #24-1

Residuals:
Number of residuals : 18
Maximum residual (m) : 2.62 at MW-31
Minimum residual (m) : -2.51 at MW-5
Residual mean (m) : 0.15
Standard deviation of residuals (m) : 1.49

Censored Data:
Number of inequalities met : 1
Number of inequalities not met : 1

WELL	MEASURED HEAD (M)	SIMULATED HEAD (M)	RESIDUAL (M)
MW-1	100.79	101.57	0.78
MW-2	104.52	103.14	-1.38
MW-3	103.07	101.26	-1.81
MW-4	<101.10	100.97	YES
MW-5	106.82	104.31	-2.51
MW-6	99.94	100.39	0.45
MW-7	101.43	102.84	1.41
MW-8	89.26	89.43	0.17
MW-9	89.34	87.53	-1.81
MW-10	<97.97	98.02	NO
MW-11		96.94	
MW-12		88.60	
MW-13		91.85	
MW-14		77.57	
MW-15		103.04	
MW-16		103.12	
MW-17	95.44	97.84	2.40
MW-18		104.80	
MW-19		95.32	
MW-20		103.14	
MW-21		94.31	
MW-22	101.02	99.54	-1.48
MW-23	70.79	71.69	0.90
MW-24		99.09	
MW-25		100.80	
MW-26	98.26	98.23	-0.03
MW-27	87.44	89.03	1.59
MW-28		98.79	
MW-29	83.30	83.14	-0.16
MW-30	82.99	85.03	2.04
MW-31	95.51	98.13	2.62
MW-32	97.63	97.80	0.17
MW-33	134.02	133.46	-0.56

FIG. X1.1 Example Listings of Residuals

Example Site
Stress scenario #2
Simulation #24-2

Residuals:
Number of residuals : 22
Maximum residual (m) : 2.30 at MW-24
Minimum residual (m) : -2.15 at MW-20
Residual mean (m) : 0.15
Standard deviation of residuals (m) : 1.22

Censored Data:
Number of inequalities met : 2
Number of inequalities not met : 0

WELL	MEASURED HEAD (m)	SIMULATED HEAD (m)	RESIDUAL (m)
MW-1	101.72	101.11	-0.61
MW-2	98.43	98.77	0.34
MW-3	100.04	100.80	0.76
MW-4	<101.10	100.57	YES
MW-5	102.95	104.45	1.50
MW-6	100.00	100.66	0.66
MW-7	101.56	102.80	1.24
MW-8	92.24	90.42	-1.82
MW-9	90.34	88.77	-1.57
MW-10	<97.97	96.88	YES
MW-11		97.69	
MW-12		90.01	
MW-13		93.43	
MW-14		80.27	
MW-15		103.58	
MW-16		103.32	
MW-17	96.33	98.62	2.29
MW-18		105.73	
MW-19		96.65	
MW-20	105.25	103.10	-2.15
MW-21	96.10	95.11	-0.99
MW-22		99.63	
MW-23	74.01	75.21	1.20
MW-24	96.66	98.96	2.30
MW-25	98.04	98.71	0.67
MW-26	97.39	98.21	0.82
MW-27	90.11	90.48	0.37
MW-28	100.23	98.76	-1.47
MW-29	84.92	84.98	0.06
MW-30	86.15	86.88	0.73
MW-31	97.87	97.38	-0.49
MW-32	97.31	97.17	-0.14
MW-33	134.43	133.96	-0.47

FIG. X1.2 Example Listings of Residuals

X1.3 Fig. X1.5 and Fig. X1.6 show sample plots of residuals in plan and cross-section, as described in 6.1.3.3. In

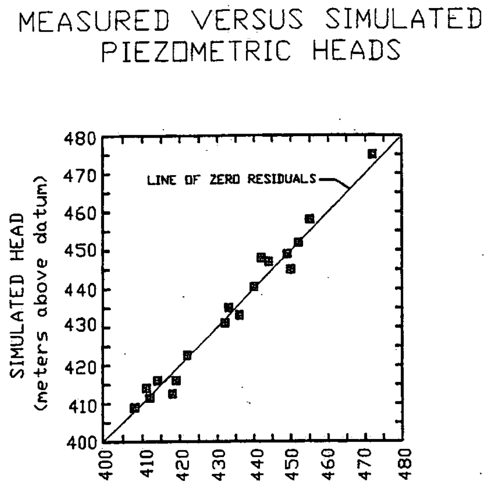

FIG. X1.3 Sample Scattergram

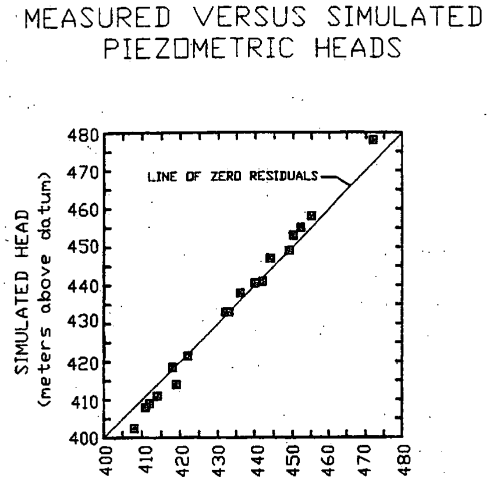

FIG. X1.4 Sample Scattergram

Fig. X1.5, there are sufficient data to contour the residuals. The contours indicate potentially significant correlations between residuals in the northwest and southwest corners of the model. Along the river, the residuals appear to be uncorrelated. In Fig. X1.6, residuals were not contoured due to their sparseness and apparent lack of correlation.

X1.4 Fig. X1.7 shows a sample plot of measured and simulated potentiometric heads and their residuals for one well in a transient simulation, as described in 6.1.3.4. The upper graph shows the measured potentiometric head at the well as measured using a pressure transducer connected to a data logger. In addition, simulated potentiometric heads for the same time period are also shown. The lower graph shows the residuals. This example shows how residuals can appear uncorrelated in a model that does not represent essential characteristics of the physical hydrogeologic system, in this case by not reproducing the correct number of maxima and minima.

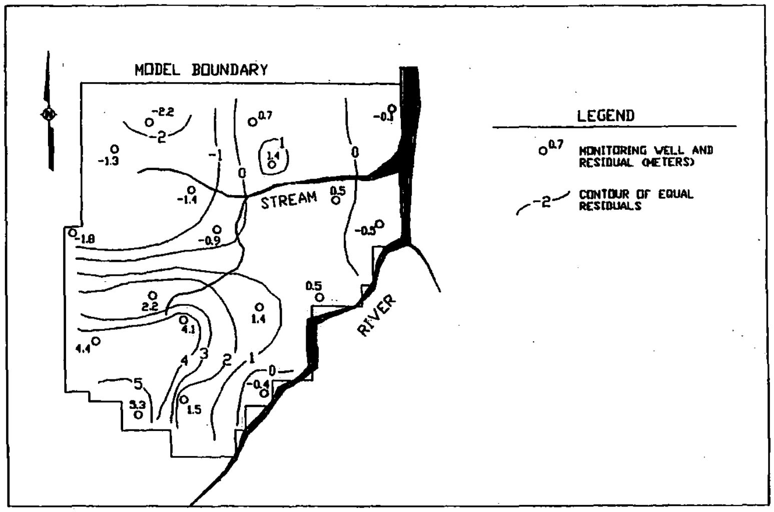

FIG. X1.5 Sample Contours of Residuals Plan View

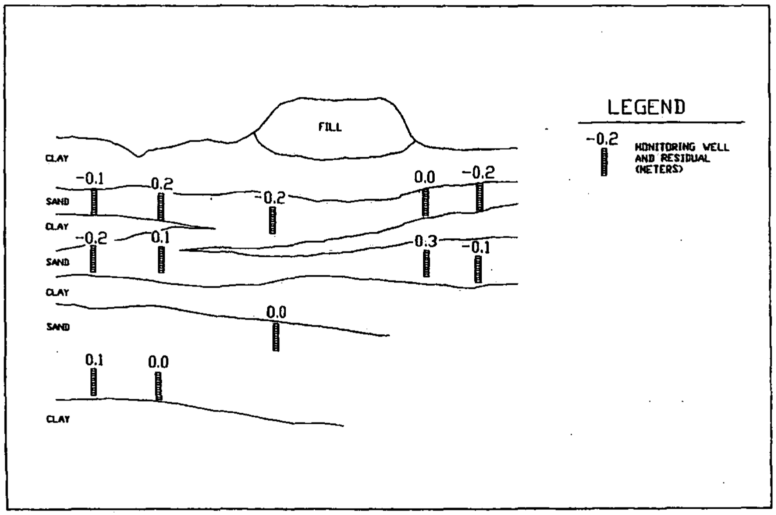

FIG. X1.6 Sample Plot of Residuals Section View

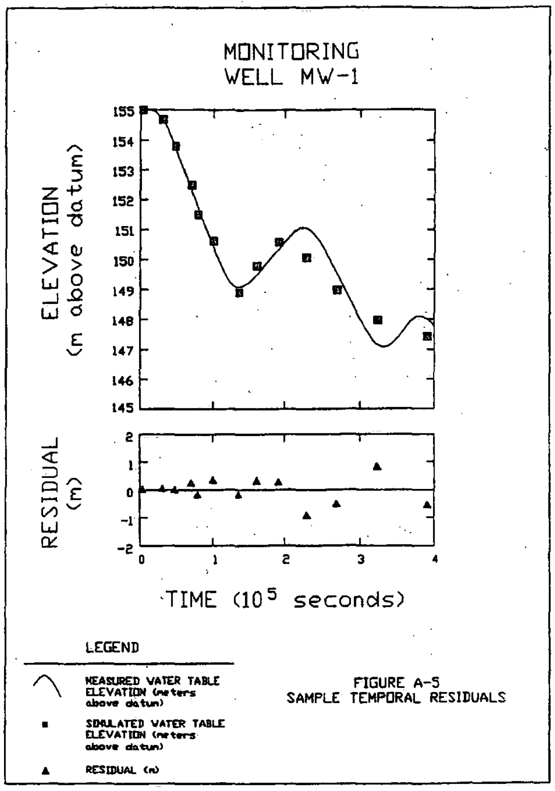

FIG. X1.7 Sample Temporal Residuals

Designation: D 5609 – 94$^{\epsilon 1}$

Standard Guide for Defining Boundary Conditions in Ground-Water Flow Modeling[1]

This standard is issued under the fixed designation D 5609; 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.

ϵ^1 NOTE—Paragraph 1.4 was added editorially October 1998.

1. Scope

1.1 This guide covers the specification of appropriate boundary conditions that are an essential part of conceptualizing and modeling ground-water systems. This guide describes techniques that can be used in defining boundary conditions and their appropriate application for modeling saturated ground-water flow model simulations.

1.2 This guide is one of a series of standards on ground-water flow model applications. Defining boundary conditions is a step in the design and construction of a model that is treated generally in Guide D 5447.

1.3 *This standard does not purport to address all of the safety concerns, 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 use.*

1.4 *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[3]

3. Terminology

3.1 *Definitions:*

3.1.1 *aquifer, confined*—an aquifer bounded above and below by confining beds and in which the static head is above the top of the aquifer.

3.1.2 *boundary*—geometrical configuration of the surface enclosing the model domain.

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

3.1.4 *conceptual model*—a simplified representation of the hydrogeologic setting and the response of the flow system to stress.

3.1.5 *flux*—the volume of fluid crossing a unit cross-sectional surface area per unit time.

3.1.6 *ground-water flow model*—an application of a mathematical model to the solution of a ground-water flow problem.

3.1.7 *hydraulic conductivity—(field aquifer tests)*, the volume of water at the existing kinematic viscosity that will move in a unit time under unit hydraulic gradient through a unit area measured at right angles to the direction of flow.

3.1.8 *hydrologic condition*—a set of ground-water inflows or outflows, boundary conditions, and hydraulic properties that cause potentiometric heads to adopt a distinct pattern.

3.1.9 *simulation*—one complete execution of the computer program, including input and output.

3.1.10 *transmissivity*—the volume of water at the existing kinematic viscosity that will move in a unit time under a unit hydraulic gradient through a unit width of the aquifer.

3.1.11 *unconfined aquifer*—an aquifer that has a water table.

3.1.12 For definitions of other terms used in this test method, see Terminology D 653.

4. Significance and Use

4.1 Accurate definition of boundary conditions is an essential part of conceptualizing and modeling ground-water flow systems. This guide describes the properties of the most common boundary conditions encountered in ground-water systems and discusses major aspects of their definition and application in ground-water models. It also discusses the significance and specification of boundary conditions for some

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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 Investigations.

Current edition approved Sept. 15, 1994. Published October 1994.

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

[3] *Annual Book of ASTM Standards*, Vol 04.09.

field situations and some common errors in specifying boundary conditions in ground-water models.

5. Types of Boundaries

5.1 The flow of ground water is described in the general case by partial differential equations. Quantitative modeling of a ground-water system entails the solution of those equations subject to site-specific boundary conditions.

5.2 *Types of Modeled Boundary Conditions*—Flow model boundary conditions can be classified as specified head or Dirichlet, specified flux or Neumann, a combination of specified head and flux, or Cauchy, free surface boundary, and seepage-face. Each of these types of boundaries and some of their variations are discussed below.

5.2.1 *Specified Head, or Dirichlet, Boundary Type*—A specified head boundary is one in which the head can be specified as a function of position and time over a part of the boundary surface of the ground-water system. A boundary of specified head may be the general type of specified head boundary in which the head may vary with time or position over the surface of the boundary, or both, or the constant-head boundary in which the head is constant in time, but head may differ in position, over the surface of the boundary. These two types of specified head boundaries are discussed below.

5.2.1.1 *General Specified-Head Boundary*—The general type of specified-head boundary condition occurs wherever head can be specified as a function of position and time over a part of the boundary surface of a ground-water system. An example of the simplest type might be an aquifer that is exposed along the bottom of a large stream whose stage is independent of ground-water seepage. As one moves upstream or downstream, the head changes in relation to the slope of the stream channel and the head varies with time as a function of stream flow. Heads along the stream bed are specified according to circumstances external to the ground-water system and maintain these specified values throughout the problem solution, regardless of changes within the ground-water system.

5.2.1.2 *Constant-Head Boundary*—A constant head boundary is boundary in which the aquifer system coincides with a surface of unchanging head through time. An example is an aquifer that is bordered by a lake in which the surface-water stage is constant over all points of the boundary in time and position or an aquifer that is bordered by a stream of constant flow that is unchanging in head with time but differs in head with position.

5.2.2 *Specified Flux or Neumann Boundary Type*—A specified flux boundary is one for which the flux across the boundary surface can be specified as a function of position and time. In the simplest type of specified-flux boundary, the flux across a given part of the boundary surface is considered uniform in space and constant with time. In a more general case, the flux might be constant with time but specified as a function of position. In the most general case, flux is specified as a function of time as well as position. In all cases of specified flux boundaries, the flux is specified according to circumstances external to the ground-water flow system and the specified flux values are maintained throughout the problem solution regardless of changes within the ground-water flow system.

5.2.2.1 *No Flow or Streamline Boundary*—The no-flow or streamline boundary is a special case of the specified flux boundary. A streamline is a curve that is tangent to the flow-velocity vector at every point along its length; thus no flow crosses a streamline. An example of a no-flow boundary is an impermeable boundary. Natural earth materials are never impermeable. However, they may sometimes be regarded as effectively impermeable for modeling purposes if the hydraulic conductivities of the adjacent materials differ by orders of magnitude. Ground-water divides are normal to streamlines and are also no-flow boundaries. However, the ground-water divide does not intrinsically correspond to physical or hydraulic properties of the aquifer. The position of a ground-water divide is a function of the response of the aquifer system to hydrologic conditions and may be subject to change with changing conditions. The use of ground-water divides as model boundaries may produce invalid results.

5.2.3 *Head Dependent Flux, or Cauchy Type*—In some situations, flux across a part of the boundary surface changes in response to changes in head within the aquifer adjacent to the boundary. In these situations, the flux is a specified function of that head and varies during problem solution as the head varies.

NOTE 1—An example of this type of boundary is the upper surface of an aquifer overlain by a confining bed that is in turn overlain by a body of surface water. In this example, as in most head-dependent boundary situations, a practical limit exists beyond which changes in head cease to cause a change in flux. In this example, the limit will be reached where the head within the aquifer falls below the top of the aquifer so that the aquifer is no longer confined at that point, but is under an unconfined or water-table condition, while the confining bed above remains saturated. Under these conditions, the bottom of the confining bed becomes locally a seepage face. Thus as the head in the aquifer is drawn down further, the hydraulic gradient does not increase and the flux through the confining bed remains constant. In this hypothetical case, the flux through the confining bed increases linearly as the head in the aquifer declines until the head reaches the level of the base of the confining bed after which the flux remains constant. Another example of a head dependent boundary with a similar behavior is evapotranspiration from the water table, where the flux from the water table is often modeled as decreasing linearly with depth to water and becomes zero where the water table reaches some specified "cutoff" depth.

5.2.4 *Free-Surface Boundary Type*—A free-surface boundary is a moveable boundary where the head is equal to the elevation of the boundary. The most common free-surface boundary is the water table, which is the boundary surface between the saturated flow field and the atmosphere (capillary zone not considered). An important characteristic of this boundary is that its position is not fixed; that is its position may rise and fall with time. In some problems, for example, flow through an earth dam, the position of the free surface is not known before but must be found as part of the problem solution.

5.2.4.1 Another example of a free surface boundary is the transition between freshwater and underlying seawater in a coastal aquifer. If diffusion is neglected and the salty ground water seaward of the interface is assumed to be static, the freshwater-saltwater transition zone can be treated as a sharp interface and can be taken as the bounding stream surface (no-flow) boundary of the fresh ground-water flow system. Under these conditions, the freshwater head at points on the interface varies only with the elevation and the freshwater head at any point on this idealized stream-surface boundary is thus a linear function of the elevation head of that point.

5.2.5 *Seepage-Face Boundary Type*—A surface of seepage is a boundary between the saturated flow field and the atmosphere along which ground water discharges, either by evaporation or movement "downhill" along the land surface as a thin film in response to the force of gravity. The location of this type of boundary is generally fixed, but its length is dependent upon other system boundaries. A seepage surface is always associated with a free surface boundary. Seepage faces are commonly neglected in models of large aquifer systems because their effect is often insignificant at a regional scale of problem definition. However, in problems defined over a smaller area, which require more accurate system definition, they must be considered.

6. Procedure

6.1 The definition of boundary conditions of a model is a part of the application of a model to a site-specific problem (see Guide D 5447). The steps in boundary definition may be stated as follows:

6.1.1 Identification of the physical boundaries of the flow system boundaries,

6.1.2 Formulation of the mathematical representation of the boundaries,

6.1.3 Examination and sensitivity testing of boundary conditions that change when the system is under stress, that is, stress-dependent boundaries, and

6.1.4 Revision and final formulation of the initial model boundary representation.

6.1.5 Further examination, testing, and refinement of the model boundaries is a part of the verification and validation process of the application of each model and is discussed in Guide D 5447.

6.2 *Boundary Identification*—Identify as accurately as possible the physical boundaries of the flow system. The three-dimensional bounding surfaces of the flow system must be defined even if the model is to be represented by a two-dimensional model. Even if the lateral boundaries are distant from the region of primary interest, it is important to understand the location and hydraulic conditions on the boundaries of the flow system.

6.2.1 *Ground-Water Divides*—Ground-water divides have been chosen as boundaries by some modelers because they can be described as stream lines and can be considered as no flow boundaries. However, the locations of ground-water divides depend upon hydrologic conditions in the sense that they can move or disappear in response to stress on the system. For these reasons, ground-water divides are not physical boundaries of the flow system.[4] Their representation as no-flow boundaries can sometimes be justified if the objective of the simulation is to gain an understanding of natural flow without applied stress or if the changed conditions used for simulation can be shown, for example, by sensitivity analysis, to have a negligible effect on the position of the boundary.

6.2.2 *Water Table*—The water table is an important boundary in many ground-water flow systems and various ways of treating the water table may be appropriate in different ground-water models. The position of the water table is not fixed and the water table boundary may act as a source or sink of water. Some of these ways of treating the water table are discussed below.

6.2.2.1 The position of the water table is not fixed, but it may be appropriate to treat the water table as a constant-head boundary in a steady-state simulation where the flow distribution in an unstressed model is simulated.

6.2.2.2 The water table may be represented as a free-surface boundary with recharge, in which case, the water table is neither a potential nor a stream surface.

6.2.2.3 The water table may be represented as a free surface boundary with discharge in which discharge is by evapotranspiration as a function of depth to water. The boundary in this case is a head-dependent flux boundary.

6.2.2.4 A sloping water table may be represented as a flow surface, that is, a locus of flow lines, where accretion is zero.

6.2.2.5 The water table may be a surface at which accretion, the net rate of gain or loss normal to the aquifer surface, is a function of time and location.

6.3 *Model Representation*—Formulate the model representation for the bounding surfaces of the flow system. Define the hydraulic conditions on the boundaries: specified head, specified flux, head-dependent flux, free surface boundary or seepage face.

6.4 *Stress Dependency*—Examine the stress-dependence of each boundary. Perform sensitivity analysis of boundaries to determine their stress dependency and to determine if natural boundaries are compatible with the representation in the model.

6.4.1 For example, a specified head boundary assumes the head is independent of the stress in the model. If the stress applied to the real system will affect the head on the boundary, the boundary is stress-dependent and modeling the boundary as a specified head boundary is not a valid representation of the boundary. Likewise, specified flux boundaries assume the flux to or from the model is independent of the stress in the model and if flux to or from the model is dependent upon head in the model, the boundary is a stress-dependent boundary and requires such recognition in representing the boundary.

6.4.1.1 Consider the physical boundary in relation to system stress to be applied during simulation. The model representation of a system boundary may be a function of the nature and magnitude of stress applied to the system during model simulation. Consider, for example, a small to medium-sized stream, which may function as a specified head boundary if the stress does not induce flow to or from the stream of sufficient magnitude to significantly affect the stream stage. If, however, the stress is so large as to cause a part of the stream to dry up, then the stream can no longer be treated as a specified head boundary. The stream may need to be modeled as a flux dependent head boundary.

6.4.1.2 If the boundary conditions are stress dependent, the

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[4] Franke, O. L., Reilly, T. E., and Bennett, G. D., "Definition of Boundary and Initial Conditions in the Analysis of Ground-Water Flow Systems—An Introduction," *Techniques of Water-Resources Investigations of the United States Geological Survey, Book 3, Chapter B5, 1987.*

model cannot be considered a general, all-purpose tool for investigating any stress on the system because it will give valid results only when the stresses do not impact the boundary. The study of a new stress on the same model may require the reformulation of the representation of boundaries of the model and sensitivity tests on the model boundary representation.

6.4.1.3 Stress-dependency is of primary concern wherever the model boundaries differ from the natural system boundaries. For example, model boundaries that may differ from physical boundaries of the flow system include natural boundaries that may extend beyond the boundaries of the model. Prepare a careful justification to show that the proposed boundary is appropriate and will not cause the model solution to differ substantially from the response that would occur in the real system.

6.5 The results of stress-dependency tests should be documented with regard to stress conditions and the magnitude of impact on stress-dependent boundaries.

6.6 *Revise Model Boundary Representation*—Based on the sensitivity testing, revise model boundary representations and document the ranges of stress for which the boundaries are designed.

7. Report

7.1 Completely document the boundary definition of the models. Such documentation will be a part of the overall documentation of the model. Include the following items pertaining to the formulation of model boundaries in the model report:

7.1.1 Describe the natural physical boundaries of the model and the processes operating at the boundaries, and

7.1.2 Describe the formulation of the model boundaries, the stress dependency of the boundaries and the model representation of each boundary. Evaluate the sensitivity analysis of the boundaries and state the conditions of stress over which the modeled boundary conditions are appropriate.

8. Keywords

8.1 aquifers; boundary condition; ground-water model

Designation: D 5611 – 94$^{\epsilon 1}$

Standard Guide for Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application[1]

This standard is issued under the fixed designation D 5611; 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.

ϵ^1 NOTE—Paragraph 1.9 was added editorially October 1998.

1. Scope

1.1 This guide covers techniques that should be used to conduct a sensitivity analysis for a ground-water flow model. The sensitivity analysis results in quantitative relationships between model results and the input hydraulic properties or boundary conditions of the aquifers.

1.2 After a ground-water flow model has been calibrated, a sensitivity analysis may be performed. Examination of the sensitivity of calibration residuals and model conclusions to model inputs is a method for assessing the adequacy of the model with respect to its intended function.

1.3 After a model has been calibrated, a modeler may vary the value of some aspect of the conditions applying solely to the prediction simulations in order to satisfy some design criteria. For example, the number and locations of proposed pumping wells may be varied in order to minimize the required discharge. Insofar as these aspects are controllable, variation of these parameters is part of an optimization procedure, and, for the purposes of this guide, would not be considered to be a sensitivity analysis. On the other hand, estimates of future conditions that are not controllable, such as the recharge during a postulated drought of unknown duration and severity, would be considered as candidates for a sensitivity analysis.

1.4 This guide presents the simplest acceptable techniques for conducting a sensitivity analysis. Other techniques have been developed by researchers and could be used in lieu of the techniques in this guide.

1.5 This guide is written for performing sensitivity analyses for ground-water flow models. However, these techniques could be applied to other types of ground-water related models, such as analytical models, multi-phase flow models, non-continuum (karst or fracture flow) models, or mass transport models.

1.6 This guide is one of a series on ground-water modeling codes (software) and their applications, such as Guide D 5447 and Guide D 5490. Other standards have been prepared on environmental modeling, such as Practice E 978.

1.7 The values stated in inch-pound units are to be regarded as the standard. The SI units given in parentheses are for information only.

1.8 *This standard does not purport to address all of the safety concerns, 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 use.*

1.9 *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[3]

D 5490 Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information[3]

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

3. Terminology

3.1 *Definitions:*

3.1.1 *boundary condition*—a mathematical expression of a

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

Current edition approved Sept. 15, 1994. Published October 1994.

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

[3] *Annual Book of ASTM Standards*, Vol 04.09.

[4] *Annual Book of ASTM Standards*, Vol 11.04.

state of the physical system that constrains the equations of the mathematical model.

3.1.2 *calibration*—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 simulations and observations of the ground-water flow system.

3.1.2.1 *Discussion*—During calibration, a modeler may vary the value of a model input to determine the value which produces the best degree of correspondence between the simulation and the physical hydrogeologic system. This process is sometimes called sensitivity analysis but for the purposes of this guide, sensitivity analysis begins only after calibration is complete.

3.1.3 *calibration targets*—measured, observed, calculated, or estimated hydraulic heads or ground-water flow rates that a model must reproduce, at least approximately, to be considered calibrated.

3.1.4 *ground-water flow model*—an application of a mathematical model to represent a ground-water flow system.

3.1.4.1 *Discussion*—This term refers specifically to modeling of ground-water hydraulics, and not to contaminant transport or other ground-water processes.

3.1.5 *hydraulic properties*—intensive properties of soil and rock that govern the transmission (that is, hydraulic conductivity, transmissivity, and leakance) and storage (that is, specific storage, storativity, and specific yield) of water.

3.1.6 *residual*—the difference between the computed and observed values of a variable at a specific time and location.

3.1.7 *sensitivity*—the variation in the value of one or more output variables (such as hydraulic heads) or quantities calculated from the output variables (such as ground-water flow rates) due to variability or uncertainty in one or more inputs to a ground-water flow model (such as hydraulic properties or boundary conditions).

3.1.8 *sensitivity analysis*—a quantitative evaluation of the impact of variability or uncertainty in model inputs on the degree of calibration of a model and on its results or conclusions.[5]

3.1.8.1 *Discussion*—Anderson and Woessner[5] use "calibration sensitivity analysis" for assessing the effect of uncertainty on the calibrated model and "prediction sensitivity analysis" for assessing the effect of uncertainty on the prediction. The definition of sensitivity analysis for the purposes of this guide combines these concepts, because only by simultaneously evaluating the effects on the model's calibration and predictions can any particular level of sensitivity be considered significant or insignificant.

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

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

4. Significance and Use

4.1 After a model has been calibrated and used to draw conclusions about a physical hydrogeologic system (for example, estimating the capture zone of a proposed extraction well), a sensitivity analysis can be performed to identify which model inputs have the most impact on the degree of calibration and on the conclusions of the modeling analysis.

4.2 If variations in some model inputs result in insignificant changes in the degree of calibration but cause significantly different conclusions, then the mere fact of having used a calibrated model does not mean that the conclusions of the modeling study are valid.

4.3 This guide is not meant to be an inflexible description of techniques of performing a sensitivity analysis; other techniques may be applied as appropriate and, after due consideration, some of the techniques herein may be omitted, altered, or enhanced.

5. Sensitivity Analysis

5.1 The first step for performing a sensitivity analysis is to identify which model inputs should be varied. Then, for each input: execute calibration and prediction simulations with the value of the input varied over a specified range; graph calibration residuals and model predictions as functions of the value of the input; and determine the type of sensitivity that the model has with respect to the input.

5.2 *Identification of Inputs to be Varied*:

5.2.1 Identify model inputs that are likely to affect computed hydraulic heads and ground-water flow rates at the times and locations where similar measured quantities exist, and thereby affect calibration residuals. Also, identify model inputs that are likely to affect the computed hydraulic heads upon which the model's conclusions are based in the predictive simulations.

5.2.2 Usually, changing the value of an input at a single node or element of a model will not significantly affect any results. Therefore, it is important to assemble model inputs into meaningful groups for variation. For example, consider an unconfined aquifer that discharges into a river. If the river is represented in a finite-difference model by 14 nodes, then varying the conductance of the river-bottom sediments in only one of the nodes will not significantly affect computed flow into the river or computed hydraulic heads. Unless there are compelling reasons otherwise, the conductance in all river nodes should be varied as a unit.

5.2.3 Coordinated changes in model inputs are changes made to more than one type of input at a time. In ground-water flow models, some coordinated changes in input values (for example, hydraulic conductivity and recharge) can have little effect on calibration but large effects on prediction. If the model was not calibrated to multiple hydrologic conditions, sensitivity analysis of coordinated changes can identify potential non-uniqueness of the calibrated input data sets.

5.3 *Execution of Simulations*:

5.3.1 For each input (or group of inputs) to be varied, decide upon the range over which to vary the values. Some input values should be varied geometrically while others should be varied arithmetically. The type of variation for each input and the range over which it is varied are based on the modeler's judgment, with the goal of finding a Type IV sensitivity (see 5.5.1.4) if it exists.

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[5] Anderson, Mary P., and Woessner, William W., *Applied Groundwater Modeling—Simulation of Flow and Advective Transport*, Academic Press, Inc., San Diego, 1992.

NOTE 1—If the value of a model input (or group of inputs) was measured in the field, then that input need only be varied with the range of the error of the measurement.

5.3.2 For each value of each group of inputs, rerun the calibration and prediction runs of the model with the new value in place of the calibrated value. Calculate the calibration residuals (or residual statistics, or both) that result as a consequence of using the new value. Determine the effect of the new value on the model's conclusions based on using the new value in the prediction simulations.

5.4 *Graphing Results*:

5.4.1 For each input (or group of inputs), prepare a graph of the effect of variation of that parameter upon calibration residuals and the model's conclusions. Figs. 1-4 show sample graphs of the results of sensitivity analyses.

5.4.2 Rather than display the effect on every residual, it may be more appropriate to display the effect on residual statistics such as maximum residual, minimum residual, residual mean, and standard deviation of residuals (see Guide D 5490).

5.4.3 In some cases, it may be more illustrative to present contours of head change as a result of variation of input values. In transient simulations, graphs of head change versus time may be presented.

5.4.4 Other types of graphs not mentioned here may be more appropriate in some circumstances.

5.5 *Determination of the Type of Sensitivity*:

5.5.1 For each input (or group of inputs), determine the type of sensitivity of the model to that input. There are four types of sensitivity, Types I through IV, depending on whether the changes to the calibration residuals and model's conclusions are significant or insignificant. The four types of sensitivity are described in the following sections and summarized on Fig. 5.

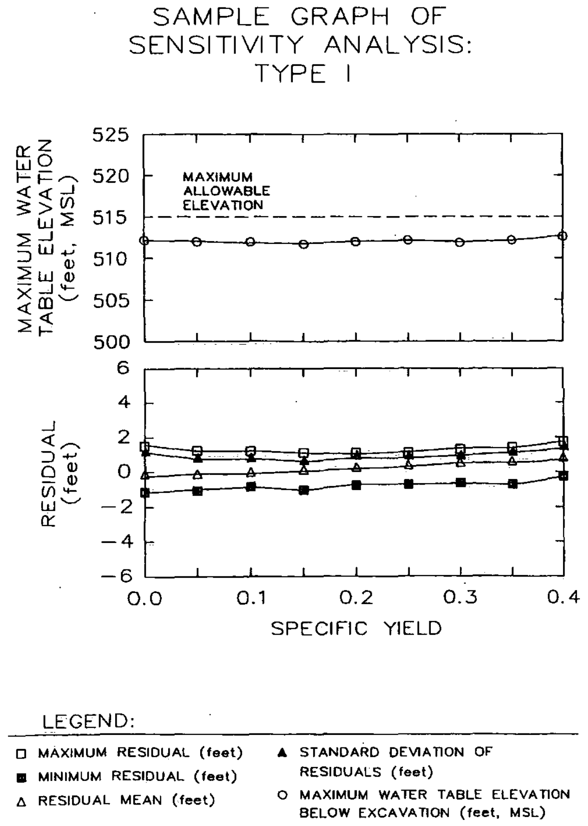

FIG. 1 Sample Graph of Sensitivity Analysis, Type I Sensitivity

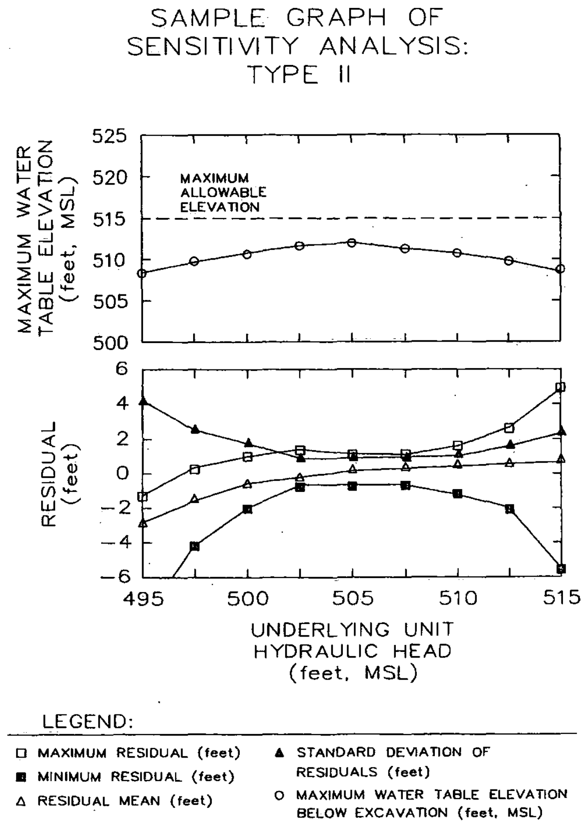

FIG. 2 Sample Graph of Sensitivity Analysis, Type II Sensitivity

NOTE 2—Whether a given change in the calibration residuals or residual statistics is considered significant or insignificant is a matter of judgment. On the other hand, changes in the model's conclusions are usually able to be characterized objectively. For example, if a model is used to design an excavation dewatering system, then the computed water table is either below or above the bottom of the proposed excavation.

5.5.1.1 *Type I Sensitivity*—When variation of an input causes insignificant changes in the calibration residuals as well as the model's conclusions, then that model has a Type I sensitivity to the input. Fig. 1 shows an example of Type I sensitivity. Type I sensitivity is of no concern because regardless of the value of the input, the conclusion will remain the same.

5.5.1.2 *Type II Sensitivity*—When variation of an input causes significant changes in the calibration residuals but insignificant changes in the model's conclusions, then that model has a Type II sensitivity to the input. Fig. 2 shows an example of Type II sensitivity. Type II sensitivity is of no concern because regardless of the value of the input, the conclusion will remain the same.

5.5.1.3 *Type III Sensitivity*—When variation of an input causes significant changes to both the calibration residuals and the model's conclusions, then that model has a Type III

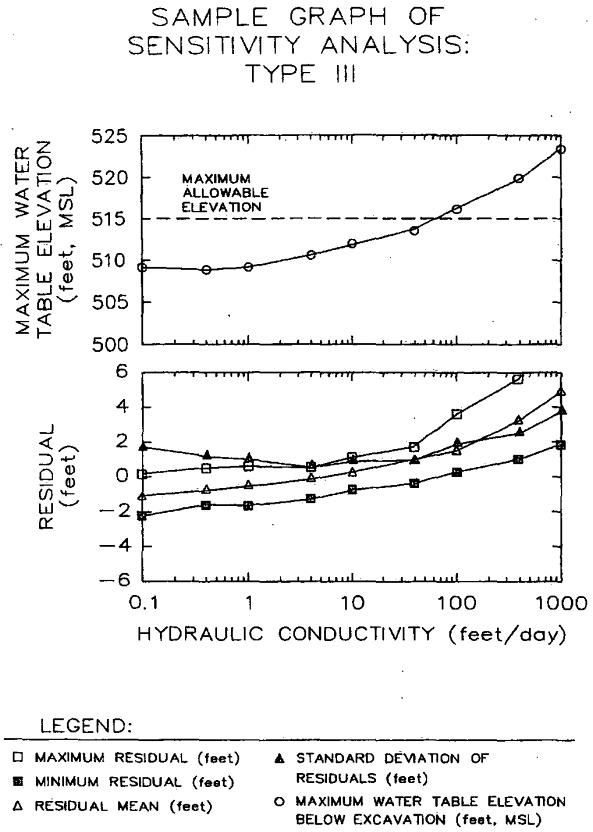

FIG. 3 Sample Graph of Sensitivity Analysis, Type III Sensitivity

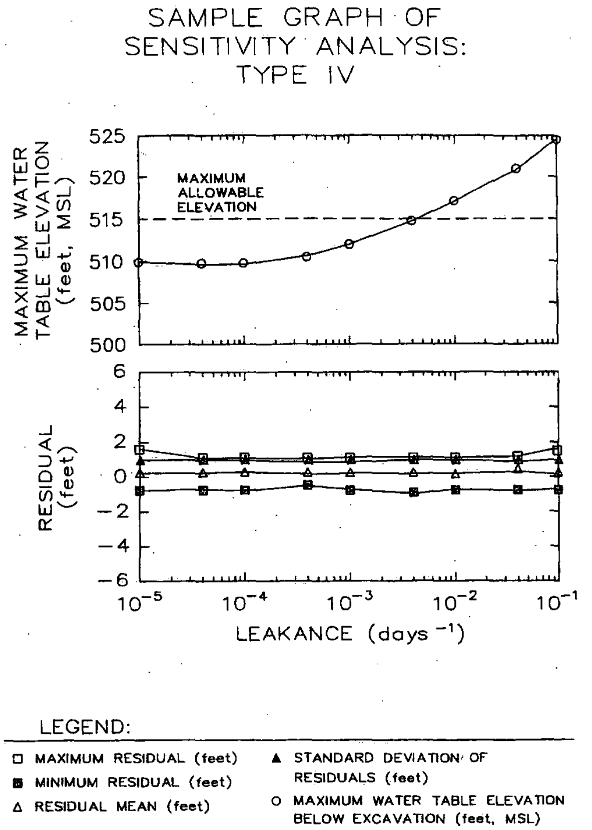

FIG. 4 Sample Graph of Sensitivity Analysis, Type IV Sensitivity

sensitivity to the input. Fig. 3 shows an example of Type III sensitivity. Type III sensitivity is of no concern because, even though the model's conclusions change as a result of variation of the input, the parameters used in those simulations cause the model to become uncalibrated. Therefore, the calibration process eliminates those values from being considered to be realistic.

5.5.1.4 *Type IV Sensitivity*—If, for some value of the input that is being varied, the model's conclusions are changed but the change in calibration residuals is insignificant, then the model has a Type IV sensitivity to that input. Fig. 4 shows an example of Type IV sensitivity. Type IV sensitivity can invalidate model results because over the range of that parameter in which the model can be considered calibrated, the conclusions of the model change. A Type IV sensitivity generally requires additional data collection to decrease the range of possible values of the parameter.

5.5.2 Some input parameters (for example, the hydraulic conductivity of a proposed cutoff wall) are used only in the prediction simulations. In such a case, the sensitivity is automatically either Type III or IV, depending on the significance of the changes in the model's conclusions. If Type IV, supporting documentation for the value of the parameter used in the prediction simulations is necessary (but not necessarily sufficient) to justify the conclusions of the model.

6. Report

CHANGE IN CONCLUSIONS	CHANGE IN CALIBRATION: INSIGNIFICANT	CHANGE IN CALIBRATION: SIGNIFICANT
INSIGNIFICANT	TYPE I	TYPE II
SIGNIFICANT	TYPE IV	TYPE III

FIG. 5 Summary of Sensitivity Types

6.1 If a sensitivity analysis is not performed, the report should state why a sensitivity analysis was not needed. If a sensitivity analysis is performed, the report should state which model inputs were varied and which computed outputs were examined. The report should justify the selection of model inputs and computed outputs in terms of the modeling objective.

6.2 For each model input that was varied, the report should present a graph showing the changes in residuals (or residual statistics) and the computed outputs with respect to changes in the model input. The report should either state that none of the analyses had a Type IV result, or else identify which analyses had Type IV results.

7. Keywords

7.1 calibration; computer; ground water; modeling; sensitivity

APPENDIX

(Nonmandatory Information)

X1. EXAMPLE SENSITIVITY GRAPHS

X1.1 Consider a hypothetical ground-water flow model used to design an excavation dewatering system. The bottom of the excavation will be at an elevation of 520 ft (158.5 m) above mean sea level (MSL), and the water table must be at least 5 feet below the excavation floor, or no more than 515 ft (157.0 m) MSL. Four parameters are selected for sensitivity analysis: the specific yield of a sand unit, hydraulic conductivity of the sand unit, the leakance of a clay unit, and the hydraulic head in an underlying silty sand unit. Figs. 1-4 show sample graphs of the results of sensitivity analyses performed on these parameters.

X1.1.1 Fig. 1 shows the results of a sensitivity analysis performed on the specific yield of the sand unit. The calibrated value was 0.2. As the specific yield was varied from 0.0 to 0.4, neither the calibration residuals nor the model conclusion varied significantly as a result of variation in the specific yield. Therefore the model has Type I sensitivity to specific yield.

X1.1.2 Fig. 2 shows the results of a sensitivity analysis performed on the hydraulic head of an underlying unit. The calibrated value was 505 ft (153.9 m) MSL. As the hydraulic head was varied from 495 to 515 ft (150.9 to 157.0 m), MSL, the residuals statistics degraded significantly. However, although the maximum water table elevation below the excavation changed, the conclusion of the model (that the excavation would stay dry) did not change. Therefore the model has Type II sensitivity to the hydraulic head in the underlying unit.

X1.1.3 Fig. 3 shows the results of a sensitivity analysis performed on the hydraulic conductivity of the sand unit. The calibrated value of the hydraulic conductivity was 10 ft (3.05 m/d) per day and it was varied from 0.1 to 1000 ft (0.03 to 304.8 m/d) per day. As the hydraulic conductivity exceeded 50 feet per day, the water table below the excavation increased to above 515 ft (157.0 m), MSL. However, the calibration residuals also increased, so that the model could no longer be considered calibrated. Therefore, the fact that the model's conclusion changed (that is, for some values of the parameter, the excavation was no longer dry) is unimportant. This is an example of Type III sensitivity.

X1.1.4 Fig. 4 shows the results of a sensitivity analysis performed on the leakance of an underlying clay unit. The calibrated value was 10^{-3} days^{-1}. As the leakance was varied from 10^{-5} to 10^{-1} days^{-1}, the calibration residuals remained practically constant. However, at the higher leakances, the excavation was not dewatered. Therefore, the conclusion of the model varied significantly while the calibration did not. This is a Type IV sensitivity, and it invalidates the use of the model for design of the excavation dewatering system until the actual value of the leakance can be determined.

X1.2 Fig. 5shows a summary of the four types of sensitivity and the conditions under which they occur.

Designation: D 5981 – 96$^{\epsilon 1}$

Standard Guide for Calibrating a Ground-Water Flow Model Application[1]

ϵ^1 NOTE—Paragraph 1.7 was added editorially October 1998.

1. Scope

1.1 This guide covers techniques that can be used to calibrate a ground-water flow model. The calibration of a model is the process of matching historical data, and is usually a prerequisite for making predictions with the model.

1.2 Calibration is one of the stages of applying a ground-water modeling code to a site-specific problem (see Guide D 5447). Calibration is 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 simulations and observations of the ground-water flow system.

1.3 Flow models are usually calibrated using either the manual (trial-and-error) method or an automated (inverse) method. This guide presents some techniques for calibrating a flow model using either method.

1.4 This guide is written for calibrating saturated porous medium (continuum) ground-water flow models. However, these techniques, suitably modified, could be applied to other types of related ground-water models, such as multi-phase models, non-continuum (karst or fracture flow) models, or mass transport models.

1.5 Guide D 5447 presents the steps to be taken in applying a ground-water modeling code to a site-specific problem. Calibration is one of those steps. Other standards have been prepared on environmental modeling, such as Guides D 5490, D 5609, D 5610, D 5611, D 5718, and Practice E 978.

1.6 *This standard does not purport to address all of the safety concerns, 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 use.*

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[3]

D 5490 Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information[3]

D 5609 Guide for Defining Boundary Conditions in Ground-Water Flow Modeling[3]

D 5610 Guide for Defining Initial Conditions in Ground-Water Flow Modeling[3]

D 5611 Guide for Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application[3]

D 5718 Guide for Documenting a Ground-Water Flow Model Application[3]

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

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, which refers to software testing, comparison with analytical solutions, and comparison with other similar codes to demonstrate that the code represents its mathematical foundations.

3.1.2 *calibrated model*—a model that has achieved a desired degree of correspondence between the model simulations and observations of the physical hydrogeologic system.

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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 04.09.

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

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 simulations and observations of the ground-water flow system.

3.1.4 *calibration targets*—measured, observed, calculated, or estimated hydraulic heads or ground-water flow rates that a model must reproduce, at least approximately, to be considered calibrated.

3.1.4.1 *Discussion*—The calibration target includes both the value of the head or flow rate and its associated error of measurement, so that undue effort is not expended attempting to get a model application to closely reproduce a value which is known only to within an order of magnitude.

3.1.5 *fidelity*—the degree to which a model application is designed to resemble the physical hydrogeologic system.

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

3.1.7 *hydraulic properties*—properties of soil and rock that govern the transmission (for example, hydraulic conductivity, transmissivity, and leakance) and storage (for example, specific storage, storativity, and specific yield) of water.

3.1.8 *inverse method*—solving for independent parameter values using knowledge of values of dependent variables.

3.1.9 *residual*—the difference between the computed and observed values of a variable at a specific time and location.

3.1.10 *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.

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

3.2 For other definitions used in this guide, see Terminology D 653.

4. Summary of Guide

4.1 The steps to be taken to calibrate a flow model are: establishing calibration targets and associated acceptable residuals or residual statistics (as described in Section 6), identifying calibration parameters (as described in Section 7), and history matching (as described in Section 8). History matching is accomplished by using the trial-and-error method to achieve a rough correspondence between the simulation and the physical hydrogeologic system, and then using either the trial-and-error method or an automated method to achieve a closer correspondence.

5. Significance and Use

5.1 Most site-specific ground-water flow models must be calibrated prior to use in predictions. In these cases, calibration is a necessary, but not sufficient, condition which must be obtained to have confidence in the model's predictions.

5.2 Often, during calibration, it becomes apparent that there are no realistic values of the hydraulic properties of the soil or rock which will allow the model to reproduce the calibration targets. In these cases the conceptual model of the site may need to be revisited or the construction of the model may need to be revised. In addition, the source and quality of the data used to establish the calibration targets may need to be reexamined. For example, the modeling process can sometimes identify a previously undetected surveying error, which would results in inaccurate hydraulic head targets.

5.3 This guide is not meant to be an inflexible description of techniques for calibrating a ground-water flow model; other techniques may be applied as appropriate and, after due consideration, some of the techniques herein may be omitted, altered, or enhanced.

6. Establishing Calibration Targets

6.1 A calibration target consists of the best estimate of a value of ground-water head or flow rate. Establishment of calibration targets and acceptable residuals or residual statistics depends on the degree of fidelity proposed for a particular model application. This, in turn, depends strongly upon the objectives of the modeling project. All else being equal, in comparing a low-fidelity to a high-fidelity model application, the low-fidelity application would require fewer calibration targets and allow larger acceptable residuals.

NOTE 1—Some low-fidelity models are not necessarily intended to make specific predictions, but rather provide answers to speculative or hypothetical questions which are posed so as to make their predictions conditional on assumptions. An example might be a model that answers the question: "If the hydraulic conductivity of the soil is 50 feet per day, will the drawdown be more than 10 ft?" This model will not answer the question of whether or not the drawdown will, in reality, be more than 10 ft because the value of hydraulic conductivity was assumed. Since the answer is conditional on the assumption, this "what-if" type of model does not necessarily require calibration, and, therefore, there would be no calibration targets.

6.2 For a medium- to high-fidelity model application, establish calibration targets by first identifying all relevant available data regarding ground-water heads (including measured water levels, bottom elevations of dry wells, and top of casing elevations of flowing wells) and flow rates (including records of pumping well or wellfield discharges, estimates of baseflow to gaining streams or rivers or recharge from losing streams, discharges from flowing wells, springflow measurements, and/or contaminant plume velocities). For each such datum, include the error bars associated with the measurement or estimate.

6.3 Establish calibration targets before beginning any simulations.

6.4 For any particular calibration target, the magnitude of the acceptable residual depends partly upon the magnitude of the error of the measurement or estimate of the calibration target and partly upon the degree of accuracy and precision required of the model's predictions. All else equal, the higher the intended fidelity of the model, the smaller the acceptable absolute values of the residuals.

6.4.1 Head measurements are usually accurate to within a few tenths of a foot. Due to the many approximations employed in modeling and errors associated therewith (see Guide D 5447), it is usually impossible to make a model reproduce all heads measurements within the errors of measurement. Therefore, the modeler must increase the range of acceptable computed heads beyond the range of the error in measurement.

Judgment must be employed in setting these new acceptable residuals. In general, however, the acceptable residual should be a small fraction of the difference between the highest and lowest heads across the site.

NOTE 2—Acceptable residuals may differ for different hydraulic head calibration targets within a particular model. This may be due to different errors in measurement, for example, when heads at some wells are based on a survey, but other heads are estimated based on elevations estimated from a topographic map. In other circumstances, there may be physical reasons why heads are more variable in some places than in others. For example, in comparing a well near a specified head boundary with a well near a ground-water divide, the modeled head in the former will depend less strongly upon the input hydraulic properties than the head in the latter. Therefore, acceptable residuals near specified head boundaries can be set lower than those near divides.

NOTE 3—One way to establish acceptable hydraulic head residuals is to use kriging on the hydraulic head distribution. Although kriging is not usually recommended for construction of hydraulic head contours, it does result in unbiased estimates of the variance (and thus standard deviation) of the hydraulic head distribution as a function of location within the modeled domain. The acceptable residual at each node can be set as the standard deviation in the hydraulic head at that location. Some researchers question the validity of this technique **(1)**.[5] An alternative is to perform trend analysis of regions of similar heterogeneity. Since a model will usually only be able to represent trends over length scales larger than the scale of local heterogeneity that is causing variations, the magnitude of the residuals from the trend analysis should approximate the magnitude of residuals in the model in that region.

6.4.2 Errors in the estimates of ground-water flow rates will usually be larger than those in heads **(2)**. For example, baseflow estimates are generally accurate only to within an order of magnitude. In such cases, the upper and lower bounds on the acceptable modeled value of baseflow can be equal to the upper and lower bounds on the estimate.

6.5 *Multiple Hydrologic Conditions*—When more than one set of field measurements have been collected, identify the different hydrologic conditions that are represented by the available data sets. Include only one data set from each hydrologic condition in the set of calibration targets. Use the remaining data sets for verification.

6.5.1 *Uniqueness (Distinct Hydrologic Conditions)*—The number of different distinct hydrologic conditions that a given set of input aquifer hydraulic properties is capable of representing is an important qualitative measure of the performance of a model. It is usually better to calibrate to multiple hydrologic conditions, if the conditions are truly distinct. Matching different hydrologic conditions is one way to address nonuniqueness, because one set of heads can be matched with the proper ratio of ground-water flow rates to hydraulic conductivities; whereas, when the flow rates are changed, representing a different condition, then the range of hydraulic conductivities that produce acceptable residuals becomes much more limited.

6.5.1.1 Other ways to address the uniqueness problem are to include ground-water flows with heads as calibration targets, and to use measured values of hydraulic properties as model inputs.

6.5.2 *Verification (Similar Hydrologic Conditions)*—When data are available for two times of similar hydrologic conditions, only one of those data sets should be used as calibration targets because they are not distinct. However, the other data set can be used for application verification. In the verification process, the modeled data are compared, not to the calibration data set, but to the verification data set. The resulting degree of correspondence can be taken as an indicator or heuristic measure of the uncertainty inherent in the model's predictions.

NOTE 4—When only one data set is available, it is inadvisable to artificially split it into separate "calibration" and "verification" data sets. It is usually more important to calibrate to data spanning as much of the modeled domain as possible.

NOTE 5—Some researchers maintain that the word "verification" implies a higher degree of confidence than the verification process imparts **(3)**. Used here, the verification process only provides a method for heuristically estimating the range of uncertainty associated with model predictions.

NOTE 6—Performing application verification protects against over-calibration. Over-calibration is the fine-tuning of input parameters to a higher degree of precision than is warranted by the knowledge or measurability of the physical hydrogeologic system and results in artificially low residuals. Without performing application verification, the artificially low residuals might otherwise be used to overstate the precision of the model's predictions.

6.6 In transient modeling, it is often easier to match changes in heads (that is, drawdowns) rather than the heads themselves. If project objectives and requirements allow, consider recasting the calibration targets as drawdowns rather than heads.

6.7 In some cases, the circumstances under which data were collected do not correspond exactly to those for which the model may be computing values. For example, the steady-state water level in a pumping well may be affected by turbulent well losses whereas the model will usually be computing the formation head at that location. To make a fair comparison and to avoid skewing calibrated hydraulic parameters to compensate for the discrepancy, either the calibration target or the computed value in the simulation should be adjusted to account for the difference. To maintain the proper perspective regarding the relative importance between measured data and modeling results, it is recommended that the computed value be adjusted prior to making the comparison, and that the calibration targets remain unaltered.

7. Identifying Calibration Parameters

7.1 Calibration parameters are groups of hydraulic properties or boundary conditions whose values are adjusted as a group during the calibration process. Examples of calibration parameters for some hypothetical model applications could be:

7.1.1 The horizontal hydraulic conductivity of a kame terrace deposit;

7.1.2 The ratio of recharge at each node in the springtime to the average annual recharge at a particular node;

7.1.3 The ground-water flux into a site in a particular corner of the model;

7.1.4 The assumed elevation of surface water in a lagoon when waste liquids were disposed of from 1969 through 1975;

7.1.5 The leakance of glacial till in an area near the toe of an earth dam; and

7.1.6 The thickness of streambed silt deposits as used to

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

calculate the leakance of river nodes.

7.2 The calibration parameters are often specified as the values of certain hydraulic properties (as in the examples in 7.1.1 and 7.1.5) or boundary conditions (as in the examples in 7.1.3 and 7.1.4) that are approximately homogeneous in space or time. In these cases, the calibration parameters are actual inputs to the flow modeling computer code. Just as often, however, calibration parameters are quantities used in the preprocessing phase of a simulation (as in the examples in 7.1.2 and 7.1.6), where other computer codes are used to create the input files for the flow modeling computer code. In these cases, use of a homogeneous calibration parameter may result in inhomogeneous inputs to the flow modeling computer code. For example, a uniform streambed thickness may result in different leakances at different river nodes due to variation in node areas.

7.3 Establish calibration parameters by identifying zones of similar aquifer hydraulic properties based on lithology, stratigraphy, and aquifer testing. Identify zones of similar recharge based on variations in surface soil type, vegetative cover, slope, and elevation. Identify other groups of inputs that can be parameterized pursuant to and consistent with project objectives.

7.4 The number of calibration parameters equals the number of degrees of freedom in a model. Ideally, this number should not exceed the number of available calibration targets. Prior information in the form of measured hydraulic properties or knowledge of the required mathematical form of the solution can relax this constraint.

7.5 For each calibration parameter, identify the range of possible realistic values that parameter may have in the physical hydrogeologic system. Establish these ranges before beginning any simulations.

8. History Matching

8.1 History matching is the part of calibration that involves varying inputs until the model simulation reproduces measured site-specific information to the desired degree of accuracy. The site-specific information can pertain to data collected during either steady-state or transient conditions. History matching is accomplished either manually, using the trial-and-error method, or automatically, using a computer program with an inverse algorithm.

8.2 Early in the calibration process it is often advisable to conduct a "calibration sensitivity analysis" by varying different inputs systematically to determine which inputs have the greatest effect on computed ground-water heads and flow rates. In early stages of calibration, this analysis allows the modeler to avoid spending time varying inputs which will have little effect on the results. In later stages of calibration, the calibration sensitivity analysis can also be used to fine-tune the input so as to minimize residuals.

NOTE 7—A "calibration sensitivity analysis" differs from a "sensitivity analysis" because the latter includes the effects of varying inputs on model predictions as well as on the calibration and therefore provides a method of distinguishing between significant and insignificant degrees of sensitivity. In contrast, the former is merely a systematic way to find the value of an input that results in the lowest residual at a point.

8.3 When comparing the results of a simulation to site-specific information, use quantitative and qualitative techniques, as described in Guide D 5490. Quantitative techniques include calculating potentiometric head residuals, assessing correlation among head residuals, and calculating flow residuals. Qualitative techniques include assessing the correspondence between the overall patterns of measured and modeled head contours, evaluating the number of distinct hydrologic conditions that a model is capable of reproducing, and assessing whether the model input parameters fall within the ranges of reasonable values previously established.

8.4 In many cases, it is possible to achieve the same degree of correspondence between simulated and measured calibration targets using different input data. This is called nonuniqueness. Since the accuracy of a prediction depends strongly on using (at least approximately) correct hydraulic conductivity values, it is necessary to resolve the nonuniqueness of the calibrated data set (**4**). This is done by using measured hydraulic conductivities or transmissivities (see 9.3), calibrating to measured ground-water flow rates as well as heads, or calibrating to data collected from multiple distinct hydrologic conditions, or both.

8.4.1 When modeling transient responses to a change in hydrologic conditions, the response in head at any point will depend primarily upon the hydraulic diffusivity of the aquifer (the ratio of the transmissivity to storativity or of hydraulic conductivity to specific storage) rather than to either hydraulic property alone. Unless one or the other property is fixed independently, a nonuniqueness in the calibrated inputs may result.

8.4.2 In a linear ground-water flow model, if all of the recharges and discharges in a model are increased by some factor and all hydraulic conductivities are increased by the same factor, the resulting computed hydraulic heads will usually remain unchanged. Unless one or the other is fixed independently, a nonuniqueness in the calibrated inputs may result.

9. Manual Calibration

9.1 The manual method of calibration is the process of changing a model input, running the modeling program with the new input, and then comparing the results of the simulation with the calibration targets. If the computed values of ground-water head and flow rate compare favorably with the measured values, then the model has been calibrated. If not, the process is repeated. This is also called the trial-and-error method.

9.2 The trial-and-error method of calibration should be used in the initial stages of calibration for all models, regardless of the method used for final calibration, although initial runs of an inverse code can give a modeler insight into fruitful directions for first calibration efforts.

9.3 When estimates of hydraulic parameters are available for the regions of the modeled physical hydrogeologic system, the corresponding values of those parameters in the model should be similar, but do not have to be identical. There are two reasons for this. First, the estimates themselves have associated errors, often of an order of magnitude. Second, when these estimates are based on hydraulic tests, the volume of soil or rock stressed by the test is often smaller than the volume in the model for which the parameter applies. In that case, the input hydraulic conductivity or transmissivity required to calibrate the model is often larger than the measured value due to the scale effect **(5)**.

9.4 Some specific suggestions for achieving a successful trial-and-error calibration follow. These techniques are strictly heuristic, and the modeler should have independent justification for such variations in input data. However, it is true that, as long as the values are reasonable for the soil or rock being modeled and the uniqueness problem is eventually addressed, the ability to match historical ground-water levels and flow rates is some justification for use of specific aquifer hydraulic properties in a model.

9.4.1 In steady state, if a particular flow line at a site begins at a specified flux boundary (for example, the no-flow boundary at an aquifer boundary or regional divide) and ends at a specified head boundary (for example, a gaining stream or river), the head at any point along the flow line depends primarily on the resistances to flow at all points between it and the specified head boundary. (This is identical to the backwater effect used by surface water hydrologists to model streamflow.) Therefore, if recharge values are not changed during the course of calibration, it is usually best to begin matching heads near the specified head boundary and then work towards the specified flux boundary.

9.4.2 When modeling transient ground-water flow, it is often advisable to begin with a steady-state scenario to calibrate the hydraulic conductivity (or transmissivity). Then, use the transient scenario to calibrate the specific storage (or storativity). This technique depends on the availability of a data set that represents approximately steady conditions in the field. (This technique is similar to, but should not be confused with, a prescription in Guide D 5447 to use the output from a calibrated steady-state model run as the initial heads for a transient simulation.)

9.4.3 To raise the hydraulic head at a point in a model, decrease the hydraulic conductivity or transmissivity, increase the recharge, decrease the conductance of the boundary nodes to which ground water at that point discharges, or increase the flow of ground water through that node, or combination thereof.

9.4.4 Speed up the response of water levels at a point to a change in boundary conditions by increasing the transmissivity or hydraulic conductivity between that area and the changed boundary, or decreasing the storativity, or specific storage in that area, or combination thereof.

9.4.5 Near a surface water body, vary the transmissivity or hydraulic conductivity to raise or lower the slope of the water table or piezometric surface and vary the conductance (or leakance) term for the boundary for the reference head to raise or lower all water levels nearby by the same amount. If the conductance term is made too large, however, the boundary will function equivalently to a constant head boundary.

9.4.6 In the vicinity of two adjacent specified head boundaries with different levels (that is, near a dam, bridge, or culvert in surface water), expect a circular component to the ground-water flow paths.

9.4.7 Increasing the leakance of a confining layer causes ground-water levels on opposite sides of a confining layer to be more equal. Decreasing the leakance can cause the levels to differ more.

9.4.8 It is usually best to begin with a simple pattern of the distribution of hydraulic properties (for example, large areas with homogeneous values) and then split some of the zones as necessary. If possible, though, avoid creating too many such zones.

9.4.9 If there are undesirable spatial correlations among residuals, try re-parameterizing the model inputs, redefining zones of equal parameter values, and smoothing transitions between zones.

9.4.10 If a model proves to be difficult to calibrate, there may be too many constant head boundaries, which would tend to overconstrain the solution. Reinvestigate the conceptual model to see whether some constant head boundaries should really be constant flux or mixed-type boundaries.

10. Automated Calibration

10.1 Automated calibration is analogous to manual calibration except that a computer code rather than the modeler adjusts model inputs or input parameters. After each simulation, the computer code compares model output against calibration targets and systematically adjusts input parameters until an objective function, based on residuals, is minimized.

10.2 There are two fundamental automated calibration techniques: direct solution and indirect solution **(6)**.

10.2.1 Direct solution uses a reformulated version of the partial differential equation of flow in which the hydraulic properties are the state variables and the hydraulic heads are the parameters and solves that equation once using numerical techniques. Direct solution requires specification of a calibration target at every node, and is generally considered to be more prone to instability than indirect solution.

10.2.2 Indirect solution iteratively improves the estimate of the inputs or input parameters until the residuals or residual statistics are acceptably small. Changes to inputs or input parameters are based on optimization or operations research techniques, most notably nonlinear least-squares optimization. Most automated calibration computer codes utilize indirect solution.

10.3 Before using automated calibration, it is often advisable to use manual calibration until the residuals or residual statistics are within an order of magnitude of the acceptable residuals or residual statistics. Using automated calibration before the model is semi-calibrated manually often results in unstable or unrealistic solutions.

10.4 For models involving a large number of input parameters, unstable or unrealistic solutions can often be avoided by estimating values for only a few of the calibration parameters at a time. It is best to begin with the parameters to which the residuals are most sensitive. For example, in a model with five hydraulic conductivity zones and three recharge zones, suppose that the residuals are more sensitive to the conductivities than to the recharge values. Then, the three recharge values would be held constant while hydraulic conductivity values are being estimated. Once the hydraulic conductivity values have been estimated, the updated hydraulic conductivity estimates are held constant and the values for the three recharge zones are estimated. After hydraulic conductivity and recharge parameters have been estimated separately, the updated values for all parameters are used as model inputs, and automated calibration is performed to determine optimal values for all parameters together. In some cases, it may be necessary to use the above technique but estimate values for one parameter at a time.

10.5 Sometimes model residuals or results, or both, are insensitive to some inputs or input parameters. These inputs or input parameters cannot be estimated using any calibration technique. Insensitive input parameters are those parameters for which a large range of values produces little change in residuals. An example would be the value of hydraulic conductivity in a small zone within a large model domain. Changing the input value for this zone may have little effect on residuals at locations that are not within or near the zone and no effect away from the zone. To assess whether the insensitivity is important in the context of the modeling objective, perform a sensitivity analysis using Guide D 5611. If the sensitivity is unimportant, remove that parameter from the list of parameters that the code is assigned to estimate.

10.6 If the automated calibration computer code allows, assign different weights to individual residuals to improve parameter estimates. For example, calibration targets associated with more precise measurements or more important locales can be given higher weights in the objective function, thereby increasing the significance of those residuals with respect to the remaining residuals. Use of weights is essential when utilizing both head and flow calibration targets in the same objective function because they have different units.

10.7 If automated calibration yields unreasonable parameter estimates, try re-parameterizing the model inputs or revisiting the conceptual model that the computer model is based upon. Some codes allow the user to assign ranges of reasonable values of each parameter, such as established in Section 7. Often, the resulting estimate for a parameter will be at one or the other limit of its allowable range. In that case, consider removing that parameter from the list of parameters that the code is assigned to estimate.

11. Report

11.1 Prepare a report (or a section of a larger report) discussing the methods used to calibrate the model. Use techniques presented in Guide D 5718.

11.2 Identify each of the calibration targets and its corresponding acceptable residual. Discuss the methods used to set the acceptable residuals.

11.3 Identify the rationale behind the choices of which model inputs were varied and which were not varied during the course of calibration.

11.4 Present quantitative and qualitative comparisons between modeled and measured information using methods presented in Guide D 5490.

12. Keywords

12.1 calibration; ground water; inverse methods; modeling; residual; trial-and-error; uniqueness; verification

REFERENCES

(1) Isaaks, E., and Srivastava, R., *Applied Geostatistics*, Oxford University Press, New York, 1989.

(2) Anderson, M. P., and Woessner, W. W., *Applied Groundwater Modeling—Simulation of Flow and Advective Transport*, Academic Press, Inc., San Diego, 1992, p 230.

(3) Konikow, L. F., and Bredehoeft, J. D., "Ground-Water Models Cannot Be Validated," *Adv. Wat. Res.*, Vol 15, 1992, pp. 75–83.

(4) Freyberg, D. L., "An Exercise in Ground-Water Model Calibration and Prediction," *Ground Water, 26(3)*, 1988, pp. 350–360.

(5) Bradbury, K. R., and Muldoon, M. A., "Hydraulic Conductivity Determinations in Unlithified Glacial and Fluvial Materials," in *Ground Water and Vadose Zone Monitoring, ASTM STP 1053*, D. M. Nielsen and A. I. Johnson, eds., ASTM, Philadelphia, 1990, pp. 138–151.

(6) Yeh, W. W-G., "Review of Parameter Identification Procedures in Groundwater Hydrology: The Inverse Problem," *Water Resources Research, 22(2)*, 1986, pp. 95–108.