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Standard Guide for Calibrating a Groundwater Flow Model Application[1]

This standard is issued under the fixed designation D5981/D5981M; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope*

1.1 This guide covers techniques that can be used to calibrate a groundwater 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 groundwater modeling code to a site-specific problem (see Guide D5447). 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 groundwater 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) groundwater flow models. However, these techniques, suitably modified, could be applied to other types of related groundwater models, such as multi-phase models, non-continuum (karst or fracture flow) models, or mass transport models.

1.5 Guide D5447 presents the steps to be taken in applying a groundwater modeling code to a site-specific problem. Calibration is one of those steps. Other standards have been prepared on environmental modeling, such as Guides D5490, D5609, D5610, D5611, D5718, and Practice E978.

1.6 *Units*—The values stated in either SI units or inch-pound units (given in brackets) are to be regarded separately as standard. The values stated in each system may not be exact equivalents; therefore, each system shall be independently of the other. Combining values from the two systems may result in non-conformance with the standard.

1.7 *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, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.8 *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.*

1.9 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

D653 Terminology Relating to Soil, Rock, and Contained Fluids
D5447 Guide for Application of a Numerical Groundwater Flow Model to a Site-Specific Problem
D5490 Guide for Comparing Groundwater Flow Model Simulations to Site-Specific Information
D5609 Guide for Defining Boundary Conditions in Groundwater Flow Modeling
D5610 Guide for Defining Initial Conditions in Groundwater Flow Modeling
D5611 Guide for Conducting a Sensitivity Analysis for a Groundwater Flow Model Application
D5718 Guide for Documenting a Groundwater Flow Model Application

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

***A Summary of Changes section appears at the end of this standard**

E978 Practice for Evaluating Mathematical Models for the Environmental Fate of Chemicals (Withdrawn 2002)[3]

3. Terminology

3.1 *Definitions:*

3.1.1 For definitions of technical terms in this standard, refer to Terminology D653.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *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.

3.2.1.1 *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.

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

3.2.2.1 *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.

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

3.2.4 *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.

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

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

3.2.7 *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.

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.

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

5. Significance and Use

5.1 Most site-specific groundwater 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 groundwater flow model; other techniques may be applied as appropriate and, after due consideration, some of the techniques herein may be omitted, altered, or enhanced.

NOTE 1—Users of the inverse method should be aware that the method may have several solutions, all equally well calibrated. (**1**)[4]

6. Establishing Calibration Targets

6.1 A calibration target consists of the best estimate of a value of groundwater 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 2—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 3 m [10 ft]?" This model will not answer the question of whether or not the drawdown will, in reality, be more than 3 m [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 groundwater 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.

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

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 D5447), it is usually not practicable 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 3—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 groundwater 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 4—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 (**2**). 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 groundwater flow rates will usually be larger than those in heads (**3**). 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 groundwater 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 groundwater 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 5—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 practicable.

NOTE 6—Some researchers maintain that the word "verification" implies a higher degree of confidence than the verification process imparts (**4**). Used here, the verification process only provides a method for heuristically estimating the range of uncertainty associated with model predictions.

NOTE 7—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