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Standard Guide for Calibrating a Ground-Water Flow Model Application¹

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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 Fluids²
- D 5447 Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem²
- D 5490 Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information²
- D 5609 Guide for Defining Boundary Conditions in Ground-Water Flow Modeling²
- D 5610 Guide for Defining Initial Conditions in Ground-Water Flow Modeling²
- D 5611 Guide for Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application²
- D 5718 Guide for Documenting a Ground-Water Flow Model Application³
- E 978 Practice for Evaluating Mathematical Models for the Environmental Fate of Chemicals⁴

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.

3.1.3 *calibration (model application)*—the process of refining the model representation of the hydrogeologic framework,

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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.

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 result 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 residuals should