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

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1. Scope

1.1 This guide covers suggested components to be included in documenting and archival of numerical ground-water flow model applications. Model documentation includes a written and graphical presentation of model assumptions and objectives, the conceptual model, code description, model construction, model calibration, predictive simulations, and conclusions. Model archival refers to a file or set of files (in both written and digital format) that contains logs of significant model simulations (that is, calibration, sensitivity and prediction simulations), supplemental calculations, model documentation, a copy of the model source code(s) or executable file(s) used, or both, and input and output data sets for significant model simulations.

1.2 This guide presents the major steps in preparing the documentation and archival for a ground-water flow model application. Additional information on ground-water model documentation can be found in EPA-500-B-92-006.[2]

1.3 This guide is specifically written for saturated, isothermal, ground-water flow model applications. The elements presented for documentation and archival are relevant and applicable to a wide range of modeled processes (in and out of the realm of ground-water flow) and can be tailored for those applications.

1.4 This guide is not intended to be all inclusive. Each model application is unique and may require supplementary documentation and archival.

1.5 *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.*

1.6 *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[3]

D 5447 Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem[4]

D 5490 Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information[4]

D 5609 Guide for Defining Boundary Conditions in Ground-Water Flow Modeling[4]

D 5610 Guide for Defining Initial Conditions in Ground-Water Flow Modeling[4]

D 5611 Guide for Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application[4]

E 978 Practice for Evaluating Environmental Fate Models of Chemicals[5]

3. Terminology

3.1 *Definitions:*

3.1.1 *application verification*—using a 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 to 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 which constrains the equations of the mathematical model.

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

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[2] *Ground-Water Modeling Compendium*, USEPA, Office of Solid Waste and Emergency Response, EPA-500-B-92-006, NTIS No. PB93207504. Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, DC, 20402.

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

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

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

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 *calibration targets*—measured, observed calculated or estimated hydraulic head or ground-water flow rates which the model must reproduce, at least approximately, to be considered calibrated.

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

3.1.6 *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.

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

3.1.8 *mathematical model*—(*a*) mathematical equations expressing the physical system and including simplifying assumptions; (*b*) the representation of a physical system by mathematical expressions from which the behavior of the system can be deduced with known accuracy.

3.1.9 *simulation log*—a log used to document (in terms of input data, code used, simulation purpose and results) of individual model simulations. (See Appendix X1.)

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

4. Significance and Use

4.1 Ground-water flow models are tools frequently applied for the analysis of hydrogeologic systems. Due to the significance of many decisions based upon modeling results, quality assurance measures need to be applied to model applications. Complete model documentation is a mechanism to ensure the quality of the effort.

4.2 Several federal and state agencies have developed policies regarding model documentation. This guide provides consistency amongst current policies, and should be used as a framework for model documentation.

5. Model Documentation

5.1 Model documentation includes written and graphical presentations of model assumptions and objectives, the conceptual model, code description, model construction, model calibration, predictive simulations, and conclusions.

5.2 *Introduction*—Present the modeling objectives, the function the model will serve, and a brief general setting of the model area. Identify the individuals involved with the modeling effort and their roles.

5.2.1 *Modeling Objectives*—Clearly state the modeling objectives, the purpose and goals of the study, and the applicability of the model as part of the study. Discuss what types of predictions are to be made with the model.

5.2.2 *Model Function*—Describe how the model was used to satisfy the purpose and goals of the study.

5.2.3 *General Setting*—Include a general setting of relevant information on the regional characteristics of topography, geology, hydrology, and land use. Present a regional map with the study area defined.

5.3 *Conceptual Model*—Present the conceptual model as a site-specific interpretation (based on collected data) of the characteristics and dynamics of the physical system being studied. Include discussion on the aquifer system (both geologic and hydrologic aspects), hydrologic boundaries, hydraulic properties, sources and sinks, and a water budget. The level of detail in this interpretation should be consistent with the available data. Present and discuss data set origins, strengths, deficiencies and their effects on the conceptual model.

5.3.1 *Aquifer System*—Present an interpretation of the geologic and hydrologic characteristics of the aquifer system. Where appropriate, present hydrogeologic cross-sections and structural contour and potentiometric surface maps to illustrate data and interpretations.

5.3.2 *Hydrologic Boundaries*—Discuss the hydrologic boundaries that exist and their type(s) for the aquifer system.

5.3.3 *Hydraulic Properties*—Present known hydraulic properties of the aquifer system, such as hydraulic conductivity, transmissivity, storativity, and porosity. If these parameters vary spatially, present the interpretation in map form.

5.3.4 *Sources and Sinks*—Present details on the location (if a point source or sink), and the relative magnitude of the source(s) or sink(s). If the source or sink is areal in extent, present information as to the variability or distribution.

5.3.5 *Water Budget*—Present a water budget (either qualitative or quantitative, depending on the study objectives) that interprets how water is entering the aquifer system, how it moves through the aquifer system, and how it exits the aquifer system.

5.4 *Computer Code Description*—Present a description of the code used and discuss the selection criteria for the code. If a custom or altered code is used, list the vendor name, any enhancements to the code, and how the code was tested. Present the simplifying assumptions inherent to the code, the limitations to the code, and the governing equations that the code solves.

5.4.1 *Assumptions*—Describe the assumptions built into the code, and justify the use of the code based on the study objectives and the conceptual model.

5.4.2 *Limitations*—Describe the limitations to the code, and the adequacy of its use based on study objectives and the conceptual model interpretation.

5.4.3 *Solution Techniques*—Describe the solution technique(s) used by the code.

5.4.4 *Effects on Model*—Describe how the assumptions and limitations of the code affect model construction, and their impact (positive or negative) on model results.

5.5 *Model Construction*—Define the model domain. Define initial conditions, boundary conditions, and hydraulic conditions, and the validity of their selection. Discuss any simplifying assumptions made to the conceptual model. Discussion should reference how the conceptual model is compatible with the modeling objectives and function. See Guide D 5610.

5.5.1 *Model Domain*—Present the model domain as an overlay on a topographic map of appropriate scale. Model grid spacing or element size should be discussed and justified based on model objectives and the conceptual model. Preprocessing and postprocessing of model data must be thoroughly documented, including any computer codes used. If the model construction is three-dimensional, describe how the layering is constructed into the model, and justify the layering based on the conceptual model.

5.5.2 *Hydraulic Parameters*—Present hydraulic parameters assigned throughout the model area. If parameter values vary spatially in the model, present this distribution in map form. Refer to the conceptual model.

5.5.3 *Sources and Sinks*—Present sources and sinks, their respective stress rates, and how they are incorporated in the model.

5.5.4 *Boundary Conditions*—Present in map form boundary conditions constructed into the model. Describe the types of boundaries, and justify their use based on the conceptual model. See Guide D 5609.

5.5.5 *Selection of Calibration Targets and Goals*—Present the calibration targets and the goals of the calibration and justify them based on the accuracy of the data used to construct the model and the study objectives.

5.5.6 *Numerical Parameters*—Present selection of any numerical parameters used in the solution technique (that is, closure criterion, acceleration, seed factor).

5.6 *Calibration*—Present and discuss model calibration procedures. Present the results of the calibration simulation in map form and compare to hydraulic head and flow data. Discuss comparison of calibration simulations to site-specific information using qualitative and quantitative techniques (see Guide D 5490). Discuss sensitivity analyses and the model verification. Discuss and present the simulation's overall water budget and mass balance. Discuss additional insight gained from the calibration regarding the conceptual model. Justify any changes made to the conceptual model. Document any preprocessing or post-processing algorithms, and any parameters these algorithms use for processing.

5.6.1 *Qualitative/Quantitative Analysis*— Describe the type of analyses used to compare calibration to site-specific data and present their results. See Guide D 5490.

5.6.2 *Sensitivity Analysis*—Present the goals of the sensitivity analysis. Document the procedures used and the results of the sensitivity analysis, and their effects on the model. Focus should be made on those parameters least well defined and most critical to the model. Justify the range of the sensitivity analyses based on the accuracy of the data. Provide the results of the sensitivity analysis in tabular or graphic form. See Guide D 5611.

5.6.3 *Model Application Verification*— Model application verification goals should be presented and discussed. Results of the verification should be presented in map form. Residuals should be presented and their significance discussed. Discuss and present the simulation's overall water budget and mass balance.

5.7 *Predictive Simulations*—Describe any predictive simulations and how they relate to the study objectives. Detail and justify the changes made to permit the calibrated model to simulate these predictions. Present results of any predictive simulations in graphical form.

5.8 *Summary and Conclusions*—Summarize the modeling effort and draw conclusions related to the study objectives. Discuss uncertainties inherent to the model and their effects on conclusions derived from the model.

5.9 *References*—Provide references for data, computer codes, and modeling procedures used as part of the modeling effort.

6. Model Archive

6.1 Maintain a model archive consisting of sufficient information generated during the modeling effort that a post-modeling audit could be adequately performed by a third party and such that future reuse of the model is possible. Components of the archive include the copies of the original data used to construct the model, simulation logs, a copy of computer codes used in the effort, a copy of the report documentation, and copies of model input and output (hard copy or digital format, or both, as appropriate) for the final calibration simulation and predictive simulations explored.

6.2 *Simulation Logs*—Archive a paper copy of the simulation log for each significant model simulation, that including the modeler's name, the simulation date, the project name/number, the simulation number, the code used (and version), the purpose of the run, the input file names, comments on the input data, the output file names, and comments on the results. An example is presented in Appendix X1.

6.3 *Computer Code*—Archive a digital copy of the executable code and if possible a copy of the source code for computer codes used in preprocessing, simulating and postprocessing. Include documentation or references for computer codes used.

6.4 *Model Documentation*—Archive a paper copy of model documentation.

6.5 *Input and Output*—At a minimum, archive model input and output for the calibration simulation, the model verification simulation, sensitivity analyses and predictive simulations.

7. Keywords

7.1 archival; documentation; ground-water model; simulation

APPENDIX

(Nonmandatory Information)

X1. MODEL SIMULATION LOG

X1.1 See Fig. X1.1.

BY ______ DATE ______
SHEET NO. ______ OF ______
PROJECT NO. ______

Simulation No. ______ Archived on Media ______

Code Used ______ Version No. ______

Purpose of Simulation: ______

Names of Input Files: ______

Comments on Input Data: ______

Names of Output Files: ______

Comments on Results: ______

FIG. X1.1 Model Simulation Log