Subsurface Fluid-Flow (Ground-Water and Vadose Zone) Modeling

Joseph D. Ritchey and
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Peer Review Policy

Each paper published in this volume was evaluated by three peer reviewers. The authors addressed all of the reviewers' comments to the satisfaction of both the technical editor(s) and the ASTM Committee on Publications.

To make technical information available as quickly as possible, the peer-reviewed papers in this publication were prepared "camera-ready" as submitted by the authors.

The quality of the papers in this publication reflects not only the obvious efforts of the authors and the technical editor(s), but also the work of these peer reviewers. The ASTM Committee on Publications acknowledges with appreciation their dedication and contribution to time and effort on behalf of ASTM.

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Foreword

This book is a collection of papers that were presented at a symposium on subsurface fluid flow (ground-water) modeling held on June 22 to 23, 1996 in Denver, Colorado. At the authors prerogative, papers were prepared for review by a minimum of three peers. The authors were then required to respond to the comments obtained in peer review. As editors we evaluated the revisions to see that they complied with the reviewers comments.

Shortly after the symposium, the editors learned of the sudden death of Jim Quinlin, one of the co-authors, and presenter of a paper. Jim was an expert in karst hydrogeology and he provided thought-provoking insights on the development and application of models of karst and fractured rock. We are thankful that Jim was able to participate in the symposium and that his co-authors were able to complete the work.

The review/revision process required a substantial amount of coordination and patience. These efforts did not go unnoticed by the editors. The twenty-four papers included in this publication involved over 72 reviews by some 40 reviewers. Our sincere appreciation to the following list of professionals:

- Tim Allen
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- Derrik Williams
- Greg Woodside

Several individuals participated in the success of the symposium and completion of this publication. These friends were task group members who have contributed through extended commitment to the standards development process. Their specific role in this publication included chairing sessions at the symposium and taking on extra reviews during the assembling of the proceedings. Our heartfelt thanks are extended to Dan Plomb, Al Laase, and Dave Brown.

ASTM has provided an important catalyst in the production of this document. Robert Morgan, D18 Staff Manger and his assistant Nancy McAvey have contributed significantly in support and communication. Dorothy Savini and her assistant Rita Hippensteel assisted greatly in symposium coordination and communication with the authors. Monica Siperko and Therese Pravitz were instrumental in bringing this document to completion. Kathy Dernoga provided key insights on resolving several difficult issues that threatened to sidetrack the document.

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Introduction

Subsurface fluid flow (ground-water) modeling serves an important role in resource development and environmental protection. This document presents newly developed methods and guidance for simulating water, air and contaminant movement in vadose and ground-water zones. This introduction provides information about the sponsoring organization, purpose, and an overview of the papers included.

Uses of models include predicting capture zones by ground-water extraction wells for water supply protection and ground-water remediation, predicting soil pore pressures due to vapor extraction, predicting the impact of air sparging on ground-water levels, and prediciting contaminant concentrations due to passive or active remediation strategies. Beyond explanation of techniques to apply ground-water models for various purposes, techniques are presented to better evaluate models or their application to available site data.

ASTM D18.21.10 on Subsurface Fluid Flow (Ground-Water) Modeling

ASTM Section D18.21.10 on Subsurface Fluid Flow Modeling is part of Subcommittee D18.21 on Ground Water and Vadose Zone Investigations, which is part of Committee D18 on Soil and Rock. D18.21.10 was formed in 1989. Section D18.21.10 has approximately 40 members, primarily from the modeling community. Although the focus of D18.21.10 is the development of standards, other forms of technology transfer, such as sponsoring symposia, are within its scope.

Sponsorship of the Symposium and Special Technical Publication 1288

The symposium and this ensuing publication were sponsored by Section D18.21.10 on Subsurface Fluid Flow Modeling, Other organizations cooperated in its presentation and preparation including the United States Environmental Protection Agency, the United States Geological Survey, and the International Ground Water Modeling Center.

Development of Standards

The standards development process began in 1989 with the formation of D18.21.10, however, the first two standards were not completed until 1991. These first standards addressed guidance on application of a ground-water flow model to a site-specific problem, and comparing site-specific data to simulation results. Since then additional standards have been prepared on defining boundary conditions, performing a sensitivity analysis, and documenting a model application. Initially these standards addressed topics on ground-water flow, however, more recently, standards have been prepared to address topics in air flow and chemical constituent movement in the subsurface.

Development of new standards is an ongoing process which includes revision and reapproval of standards that have already been published. ASTM society rules require periodic reapproval of standards. This is an important part of the process because it mandates that standards remain current and reflective of changes in technology. If a standard is not reapproved, it is removed from all ASTM publications. This is part of the normal life-cycle of standards.

Terminology

Establishing a consistent set of terminology is an integral part of standards development. Discussion about the use of certain terms may never reach a consensus, whereas some other terms have never needed much debate. ASTM standards include a section on terminology specific to the standard. Additionally, one of the six types of ASTM standards is terminology. The ASTM standard terminology which includes terms on the vadose zone and ground water is D653.

The term ground water is the subject of much controversy, to a small extent its definition, but a larger extent its spelling. The controversy on the spelling of ground water centers on whether it should be one or two words. Within ASTM and several other major organizations including the USGS and the National Ground Water Association, ground water is two words, hyphenated when used as an adjective. That is the preferred use within this document, however, we did not reject papers on the basis of how ground water was spelled.

In D653 the term ground water is defined as "water that occurs beneath the earth's surface in the saturated zone". The original title for Section D18.21.10 was "Ground-water Modeling"; however, due to the limitations on what constitutes ground water in ASTM, the title was changed to "Subsurface Fluid Flow Modeling". Voids in the rock beneath the surface, both in the vadose zone and the zone of saturation, may contain ground water, however, other fluids may also be present such as chemical contaminants like gasoline or solvents. Of course air is present in the vadose zone, but not necessarily with the chemical composition that we are accustomed to in the atmosphere. Other natural and artificially induced gases may also be present. As an example, carbon dioxide is produced by biologic activity in the destruction of organic matter.

Overview

The purpose of the symposium and this publication was to provide an open forum for expression of innovative methods in applying models. Model codes are discussed, for the most part, as a integral component of the application. Several papers are included that discuss comparison of several codes to a single data set.

Organization of the symposium and of this document conforms to the sequence of steps that make up the modeling process. The 24 papers included have been grouped into the six steps. The process is also described in ASTM D5747 and here it is discussed by Woessner and Anderson.

By taking on this format, this document provides a logical progression for the novice modeler. Beyond this, the document provides important information for the experienced modeler by presenting previously unpublished results of research and applications.

Assessment of Modeling

Modeling begins with a definition of the problem and establishment of data available to support a solution. These items can be thought of as the architects plan for a building and the available materials. Four papers are included in this section.

The first paper, by Lee et.al., is a review of twenty model application reports. In a sense this paper is like a compilation of a building inspector's observations. Candidly, the inspector was not pleased with the results and recommendations are presented that may help rectify the situation in the future.

The second paper, by Woessner and Anderson, looks at the overall modeling process. The authors propose that ground-water modeling is inherently uncertain, acceptability of a modeling effort is based on the number and strength of confirming observations, and that a subjective judgment will always be required to determine if a model appropriately represents the ground water system. Among their conclusions is that additional standardization of modeling efforts will not preclude the need for subjective judgment during the process.

The third paper, by Brown, acknowledges the uncertainty discussed by Woessner and Anderson and provides additional in-sights on steps to reduce it. Brown high-lights ASTM standards that can be used to aid in reducing uncertainty in the modeling process. An example of a topic discussed by Brown is the lack of uniqueness when a single set of measured water levels are used in calibration of a flow model. Brown follows with three ways to address uniqueness in a model application.

The fourth paper, by Hansen, considers model codes that are prepared for general use. The codes require input of simulation definition, material properties, and boundary and initial conditions. Few codes utilize standard or uniform input data sets for information that for the most part is identical for models of like dimensionality. Geographical Information Systems (GIS) provide a method to organize, manipulate, and analyze data much beyond the requirements of models. The United States federal government has adopted Content Standards for Digital Geospatial Metadata.

Conceptualization

Solution to every subsurface flow problem always includes some act of conceptualization. Proper conceptualization is essential to obtaining good model results. This step and its interrelation to site characterization is in the first paper by Kolm, et.al. First, in our consideration of a modeling application is site characterization and conceptualization. The three papers that follow address specific hydrologic or geologic settings: an alluvial basin, a recharge sensitive valley-fill aquifer, and an unconfined carbonate aquifers. Overall, the four papers provide helpful information applicable to all modeling and some specific observations over a wide range of geologic settings.

Conceptualization and characterization of ground-water flow systems is described by Kolm, et.al.. The authors describe key steps including establishing a scope and scale of the model, problem definition, data base development, and surface, geologic, and geomorphic characterization. This broad treatment of the subject is followed by Williams et.al. who describe evaluation of a previously accepted conceptual model and their development of a new model. The paper describes conceptualization of a complex multilayer system and efforts to reconcile differences between past and current models. Williams and Morrissey present an examination of the role of upland runoff as a major source of recharge to many glacial valley-fill aquifers. Three valley-fill aquifer models are described along with the methods used to estimate and represent recharge.

Conceptualization of ground-water systems where formations are composed of carbonate rocks may be extremely difficult because the range of complexity can be so radical. Quinlan et.al. address the applicability of numerical models to aquifers composed of soluble rocks. The authors discuss design requirements and boundary conditions. This information is a compelling reality check when considering applying a porous medium code to fractured or solutioned aquifers.

Code Selection/Validation

The next step is selecting and validating the model code that best fits the model objectives and is consistent with the results of the conceptual model. The four papers in this section describe several model codes and how they compare when applied to similar data sets.

Delineation of capture zones for wellhead protection can be computed using several techniques. Green and Dorrler compare calculated capture zones by three general techniques; calculated fixed radius, analytical equations, and numerical modeling. As expected, numerical modeling was most data demanding and provided the most representative results, however, simpler techniques were not consistent in providing "conservative" solutions.

A similar approach is taken by Rowe and Nadarajah, who discuss cross-checking solute transport model results using analytic, finite layer, and finite element methods. Mummert discusses use of point validation and statistical validation of a previously developed model to simulate nitrate percolation from land application of sewage sludge.

Model Design and Construction

Within the ground-water modeling process, design and construction includes establishing the model grid and boundary conditions and conducting simulations sufficient to show that the code is operating correctly.

This step includes many substeps that depending on the complexity of the application and of the code can be painless or painful. The six papers are included in this section to demonstrate the diversity of codes and applications and to provide the user with options to simplify the process. Thrupp et.al describe application of ground-water flow modeling to unsaturated soils to evaluate performance of a soil vapor extraction system.

Three papers present overviews of model codes that have been integrated with graphical user interfaces or include pre and post processors. The Department of Defense Groundwater Modeling System, described by Holland, is an integrated comprehensive ground-water flow and solute transport modeling system. Eddebbarh et.al., describes use of the Micro-Fem software for constructing the model data set; the results are compared to the MODFLOW code. Heinzer et.al. describes a graphical user interface developed for use with geographical information system data and the USGS MODFLOW code.

Two final papers in this section describe design of a multi-model application of flow and transport and modeling multiphase flow. McNulty et.al discuss design of a fate and transport model that included infiltration and mixing of contaminated surface runoff. Lundegard and Andersen present an application of a multiphase flow model to simulate air sparging of ground water.

Calibration

Although the calibration step is not required for every model use, it is a critical part of most model applications. Calibration is the act of adjusting uncertain model input parameters within reasonable limits to achieve an acceptable correspondence between observed and measured output. The calibration step includes sensitivity analysis. The first paper, by Laase and Davidson, describes a method for assessing the correspondence between simulated and measured output. The second paper, by Baker et.al., presents a automated calibration procedure following a systematic trial and error method.

Application Verification/Uncertainty

With satisfactory completion of calibration process, the model should be verified for the intended use of the application. The first paper, by Johnson and Weimer, describes the use of water level data from three different time periods, cumulative water recovery volumes from well and trench extraction systems located in different areas, and infiltration tests at two different locations in verification of a ground-water model application. The second paper, by Fermor et.al., describes a procedure of conducting multiple simulations of plausible combinations of model parameters, rejecting implausible catchments, and evaluating a confidence index. The third paper, by Ruskauff, discusses a geostatistical analysis of hydraulic conductivity. The methodology applied shows how to circumvent obstacles in the analysis.

Post Audit

The post audit is a desirable step which is rarely performed. The purpose of the post audit is to test the model predictions against reality, thus verifying the model predictions. Most model applications end with predictive simulations. However, as in the case described by Weaver et.al., investigation of a site often progresses to design of a remediation system and the application of a second modeling phase to predict the aquifer response to the remedial action. The presentation by Weaver et.al. serves as an example of a post audit and gives insight into the model design process.

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