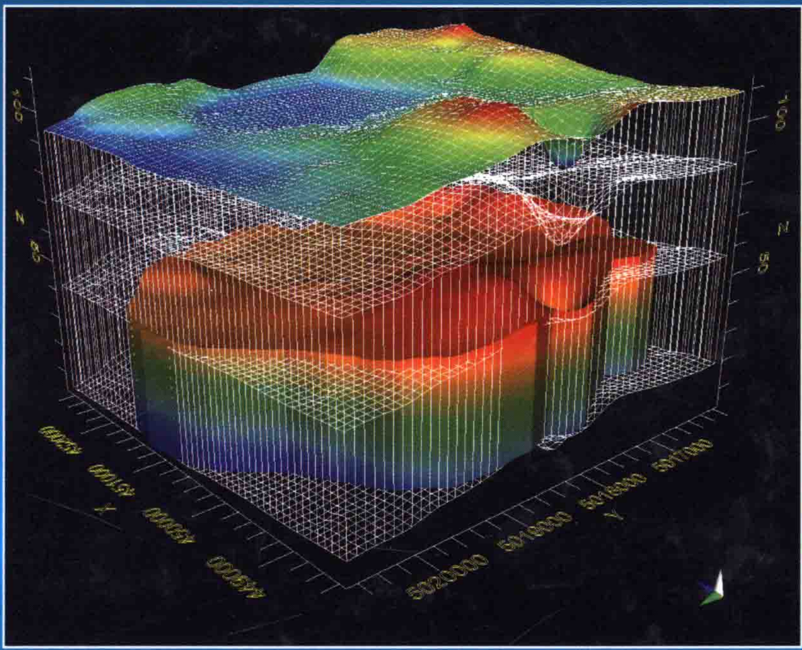
Second Edition

Applied Groundwater Modeling

Simulation of Flow and Advective Transport



Mary P. Anderson
William W. Woessner
Randall J. Hunt

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Simulation of Flow and Advective Transport

Second Edition

MARY P. ANDERSON

Department of Geoscience, University of Wisconsin-Madison, Madison, Wisconsin

WILLIAM W. WOESSNER

Department of Geosciences, University of Montana, Missoula, Montana

RANDALL J. HUNT

U.S. Geological Survey, Wisconsin Water Science Center, Cross Plains, Wisconsin

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The front cover image is provided courtesy of Schlumberger Water Services. The image represents a uniform grid for a multi-layer finite-difference MODFLOW model and was produced using the software Visual MODFLOW Flex. Colors at the top of the image represent changes in land surface elevation; colors in the bottom layers represent geologic variability. The back cover graphic is a word cloud created using all text contained in Chapters 1−12. Word-cloud graphics included with the introductory sections of the book consist of text contained in each section. All word clouds were generated using Wordle, created by Jonathon Feinberg (www.wordle.net).

APPLIED GROUNDWATER MODELING

...to Charles, Jean, and Lori

PREFACE

Art and science have their meeting point in method.

Edward George Bulwer-Lytton

This second edition is motivated by the many significant developments in groundwater modeling since the first edition was published in 1992. The increased computational speed and capacity of present day multicore computers as well as the availability of sophisticated graphical user interfaces (GUIs) and geographical information systems have transformed groundwater modeling. But more importantly, new ways of calibrating models and analyzing uncertainty and new powerful codes that provide enhanced modeling tools are revolutionizing the science of groundwater modeling. In this second edition, we discuss many of the important advances in applied groundwater modeling introduced since 1992 and also update the treatment of fundamentals of groundwater flow modeling covered in the first edition. The chapters on model calibration and forecasting (Chapters 9 and 10 in the second edition) are entirely new and include discussion of new tools for parameter estimation and uncertainty analysis in forecast simulations. Similar to the first edition, our book is intended as an introduction to the applied science of modeling groundwater flow. We focus on groundwater modeling practice. For a more theoretical approach to groundwater modeling, the reader is referred to textbooks by Diersch (2014) and Bear and Cheng (2010).

Quantitative analysis of groundwater flow is essential to all hydrogeological problems, and groundwater models are the essential tools in such analyses. Groundwater flow models solve for what cannot be fully observed or measured—the distribution of head in space and time. Important associated information such as water budgets, flow rates, and flowpaths to and from surface water bodies and wells can be calculated from the head distribution. The focus of our book is mastering groundwater flow models, a critical first step for a groundwater modeler.

Although many groundwater problems can be solved by analyzing groundwater flow alone, some problems require analysis of the movement of solutes or contaminants in the subsurface. A transport model includes representation of advective transport, dispersion, and chemical reactions to solve for solute or contaminant concentrations. Transport modeling is beyond the scope of our textbook but is covered in detail by Zheng and Bennett (2002). However, the starting point for transport modeling is a good groundwater flow model because a transport code uses output from a groundwater flow model. Moreover, some transport problems can be addressed by considering only advective transport using a particle tracking code as a postprocessor to a groundwater flow model to calculate flowpaths and travel times. We discuss those types of problems in a chapter on particle tracking (Chapter 8 in the second edition) that was revised and updated from the first edition.

Mastery of groundwater modeling requires both art and science. The science of groundwater modeling includes basic modeling theory and numerical solution methods. There are many textbooks that provide advanced, intermediate, and elementary treatments of the science and underlying mathematics of numerical modeling of groundwater flow. Since 1992, applied groundwater science has expanded to include theory and methods for parameter estimation (inverse solutions) and uncertainty analysis, and there are books devoted exclusively to those topics (e.g., Doherty, 2015; Aster et al., 2013; Hill and Tiedeman, 2007). Although our text provides some of the background information for applying groundwater models to field problems, we assume that the reader knows the basic principles of hydrogeology and modeling as covered in standard textbooks such as Fitts (2013), Kresic (2007), Todd and Mays (2005), Schwartz and Zhang (2003), and Fetter (2001). A rudimentary knowledge of the theory of groundwater modeling including the basics of finite-difference and finite-element methods as contained in Wang and Anderson (1982) is also helpful.

Our book is meant to be accessible to those who want to apply groundwater models as tools. To use an analogy presented to us years ago by Professor John Wilson (New Mexico Tech), using a model is like driving a car. A good driver knows the rules of the road and has the skill to control the car under a wide variety of conditions and avoid accidents, but does not necessarily understand the intricacies of what goes on under the hood of the car. The goal of this book is to help the reader learn how to be a good driver and operate a model under a wide variety of conditions and avoid "accidents." To help in this, we have included a section at the end of each chapter in which we list common modeling errors—some we have encountered and many we have made ourselves. Eventually, after learning how to drive well, a modeler may want to explore the mechanics of a code (i.e., look under the hood of the car); familiarity with code mechanics helps the modeler understand the strengths and limitations of a specific code and will help the modeler modify the code if necessary.

The art of modeling is gained mainly through experience; by developing and applying groundwater models one develops "hydrosense" and modeling intuition (Hunt and Zheng, 2012). Our book provides guidance in the fundamental steps involved in the art of modeling: developing a conceptual model, translating the qualitative conceptual model to a quantitative (numerical) model, and assessing model input and output. Given that "art and science have their meeting point in method," our objective is to describe methods of applying groundwater flow models, and thereby provide a compact comprehensive reference to assist those wishing to develop proficiency in the art of modeling.

The book comprises four sections. Section 1, Modeling Fundamentals (Chapters 1, 2, and 3), lays out the motivation for modeling, describes the process of formulating a conceptual model, and provides the theoretical and numerical base. Section 2, Designing the

Numerical Model (Chapters 4 through 7), describes how to translate the conceptual model of groundwater flow into a numerical model, including grid/mesh design, selecting boundary and initial conditions, and setting parameter values. Section 3, Particle Tracking, Calibration, Forecasting, and Uncertainty Analysis (Chapters 8 through 10) discusses particle tracking and model performance. Section 4, The Modeling Report and Advanced Topics (Chapters 11, 12) discusses the modeling report and archive, model review, and briefly covers topics beyond basic groundwater flow modeling.

In the first edition, we made extensive reference to specific flow and particle tracking codes to illustrate examples of modeling mechanics. However, the number and capabilities of groundwater codes have increased dramatically since 1992. In the second edition, we illustrate how fundamental modeling concepts are implemented in two representative groundwater flow codes: MODFLOW (for finite-difference methods) and FEFLOW (for finite-element methods). We use MODFLOW (http://water.usgs.gov/ogw/modflow/MODFLOW.html) because it is freeware, open-source, well-documented, versatile, used worldwide and in the US is the standard code in regulatory and legal arenas. The proprietary code FEFLOW is widely used, versatile, well-supported, and well-documented both online (http://www.feflow.com/) and in a textbook (Diersch, 2014). We selected the PEST software suite (http://www.pesthomepage.org) to illustrate how concepts of parameter estimation can be implemented. The PEST suite of codes (Doherty 2014, 2015; Welter et al., 2012; Fienen et al., 2013) is freeware and open-source, includes widely used approaches for parameter estimation with many advanced options. A version of PEST (PEST++ by Welter et al., 2012) is supported by the U.S. Geological Survey (http://pubs.usgs.gov/tm/tm7c5/). In practice, the modeler will typically use these codes within a GUI. The details of how the codes work within a GUI are not covered in our book. The reader should expect to spend practice time with a GUI to be accomplished in using these or any other codes.

The many new developments and advances in groundwater modeling since the first edition are supported by an enormity of literature. Therefore, we developed some general guidelines for presentation of material in the second edition.

- We focus on "the norm" rather than "the exception" in order to guide the reader to the most likely productive approach for most problems.
- We use language and mathematics accessible to the beginning and intermediate level groundwater modeler and try to avoid jargon. Necessarily, the advanced modeler may find our presentation at times overly simple or lacking in rigor.
- For the most part, we reference widely available software; the vast majority of applied groundwater modeling is done with off-the-shelf software.
- We recognize that software, jargon, and methods will change in the future. Therefore, our text focuses on the basic principles of groundwater modeling that will endure. However, we use code-specific language and variable names when we believe that such specificity is beneficial.

- We mainly cite work published in the twenty-first century, as well as classic (benchmark) papers. References cited should be regarded as portals into the large body of pertinent literature on a specific topic. That is, the provided reference is cited not only for itself but also for all the work cited therein. In this way, the reader is given the opportunity to consult a broad body of literature and explore a research thread. Reports published by the U.S. Geological Survey are available for free download at http://www.usgs.gov or at the provided Universal Resource Locators (URLs).

With the maturing of the science, groundwater modeling has become more interdisciplinary and relevant publications are distributed across a wide variety of journals. No textbook can fully cover all the relevant literature. Therefore, we apologize in advance to those who may feel we have overlooked their contributions.

The second edition has an associated Web site that will contain background material, example problems, and links to other modeling resources (http://appliedgwmodeling.elsevier.com). We hope this material, together with the textbook, will be useful on two levels: (1) for teaching undergraduate and graduate level courses in applied groundwater modeling; (2) as a reference for environmental consultants and those in industry and governmental agencies. In its broadest intent, our book is meant for those who want to learn how to build, use, and assess groundwater flow models. We hope that reading this book will facilitate a life-long journey in groundwater modeling.

All things are ready, if our minds be so.

—Henry V, Act IV

Mary P. Anderson, Madison, Wisconsin
William W. Woessner, Missoula, Montana
Randall J. Hunt, Cross Plains, Wisconsin

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DISCLAIMER

The material in this book is intended to guide those familiar with the basics of hydrogeology and groundwater flow modeling in developing numerical groundwater flow models of field problems. Although the information in this book is presented in the belief that it will help the reader to minimize errors, no responsibility is assumed by the authors, the U.S. Government and other institutions with which the authors are affiliated, or the publishers for any errors, mistakes, or misrepresentations that may occur from the use of this book, and no compensation will be given for any damages or losses whatever their cause.

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I can no other answer make but thanks,
And thanks, and ever thanks

—Twelfth Night, Act III, Scene III