EFFECTIVE GROUNDWATER MODEL CALIBRATION

With Analysis of Data, Sensitivities, Predictions, and Uncertainty

MARY C. HILL
CLAIRE R. TIEDEMAN

WILEY-INTERSCIENCE
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We dedicate this book to the groundwater modelers and software developers of the U.S. Geological Survey. These men and women devote their careers to providing sound scientific analyses for policy makers and to enabling others in the government and the private sector to do the same. We are honored to be their colleagues.

We also dedicate this book to the United States taxpayers, to whom we are ultimately accountable. They have supported our educations, salaries, field work and students. We hope our efforts have improved the understanding and management of their groundwater resources.

With love, we also dedicate this book to our husbands and families.

CONTENTS

PREFACE

This book is intended for use in undergraduate and graduate classes, and is also appropriate for use as a reference book and for self-study. Minimal expertise in statistics and mathematics is required for all except a few advanced, optional topics. Knowledge of groundwater principles is needed to understand some parts of the exercises and some of the examples, but students from other fields of science have found classes based on drafts of the book to be very useful.

This book has been more than 12 years in the making. Progressively more mature versions have been used to teach short courses most years since 1991. The short courses have been held at the U.S. Geological Survey National Training Center in Denver, Colorado; the International Ground Water Modeling Center at the Colorado School of Mines in Golden, Colorado; the South Florida Water Management District in West Palm Beach, Florida; the University of Minnesota, in Minneapolis, Minnesota; the Delft University of Technology, The Netherlands; Charles University in Prague, the Czech Republic; University of the Western Cape in Belleville, South Africa; and Utrecht University, The Netherlands. A version also was used to teach a semester course at the University of Colorado in Boulder, Colorado in the fall of 2000. Much of what the book has become results from our many wonderful students. We thank them for their interest, enthusiasm, good humor, and encouragement as we struggled to develop many of the ideas presented in this book.

We also are deeply indebted to the following colleagues for insightful discussions and fruitful collaborations: Richard L. Cooley, Richard M. Yager, Frank A. D'Agnese, Claudia C. Faunt, Arlen W. Harbaugh, Edward R. Banta, Marshall W. Gannett, and D. Matthew Ely of the U.S. Geological Survey, Eileen P. Poeter of the Colorado School of Mines, Evan R. Anderman formerly of Calibra Consultants and McDonald-Morrissey Associates, Inc., Heidi Christiansen Barlebo of the

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All errors and omissions are the sole responsibility of the authors.

Mary C. Hill
Claire R. Tiedeman

1

INTRODUCTION

In many fields of science and engineering, mathematical models are used to represent complex processes and results are used for system management and risk analysis. The methods commonly used to develop and apply such models often do not take full advantage of either the data available for model construction and calibration or the developed model. This book presents a set of methods and guidelines that, it is hoped, will improve how data and models are used.

This introductory chapter first describes the contributions of the book, including a description of what is on the associated web site. Sections 1.2 and 1.3 provide some context for the book by reviewing inverse modeling and considering the methods covered by the book relative to other paradigms for integrating data and models. After providing a few definitions, Chapter 1 concludes with a discussion of the expertise readers are expected to possess and some suggested readings and an overview of Chapters 2 through 15.

1.1 BOOK AND ASSOCIATED CONTRIBUTIONS: METHODS, GUIDELINES, EXERCISES, ANSWERS, SOFTWARE, AND POWERPOINT FILES

The methods presented in the book include (1) sensitivity analysis for evaluating the information content of data, (2) data assessment strategies for identifying (a) existing measurements that dominate model development and predictions

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and (b) potential measurements likely to improve the reliability of predictions, (3) calibration techniques for developing models that are consistent with the data in some optimal manner, and (4) uncertainty evaluation for quantifying and communicating the potential error in simulated results (e.g., predictions) that often are used to make important societal decisions.

The fourteen guidelines presented in the book focus on practical application of the methods and are organized into four categories: (1) model development guidelines, (2) model testing guidelines, (3) potential new data guidelines, and (4) prediction uncertainty guidelines.

Most of the methods presented and referred to in the guidelines are based on linear or nonlinear regression theory. While this body of knowledge has its limits, it is very useful in many circumstances. The strengths and limitations of the methods presented are discussed throughout the book. In practice, linear and nonlinear regression are best thought of as imperfect, insightful tools. Whether regression methods prove to be beneficial in a given situation depends on how they are used. Here, the term beneficial refers to increasing the chance of achieving one or more useful models given the available data and a reasonable model development effort. The methods, guidelines, and related exercises presented in this book illustrate how to improve the chances of achieving useful models, and how to address problems that commonly are encountered along the way.

Besides the methods and guidelines, the book emphasizes the importance of how results are presented. To this end, the book can be thought of as emphasizing two criteria: valid statistical concepts and effective communication with resource managers. The most advanced, complex mathematics and statistics are worth very little if they cannot be used to address the societal needs related to the modeling objectives.

The methods and guidelines in this book have wide applicability for mathematical models of many types of systems and are presented in a general manner. The expertise of the authors is in the simulation of groundwater systems, and most of the examples are from this field. There are also some surface-water examples and a few references to other fields such as geophysics and biology. The fundamental aspects of systems most advantageously addressed by the methods and guidelines presented in this work are those typical of groundwater systems and shared by many other natural systems. Of relevance are that groundwater systems commonly involve (1) solutions in up to three spatial dimensions and time, (2) system characteristics that can vary dramatically in space and time, (3) knowledge about system variability in addition to the data used directly in regression methods, (4) available data sets that are typically sparse, and (5) nonlinearities that are often significant but not extreme.

Four important additional aspects of the book are the exercises, answers, software, and PowerPoint files available for teaching.

The exercises focus on a groundwater flow system and management problem to which students apply all the methods presented in the book. The system is simple, which allows basic principles to be clearly demonstrated, and is designed to have aspects that are directly relevant to typical systems. The exercises can be conducted using the material provided in the book, or as hands-on computer exercises using instructions and files available on the web site http://water.usgs.gov/lookup/get?crresearch/hill_tiedeman_book.

The web site includes instructions for doing the exercises using files directly and/or using public-domain interface and visualization capabilities. It may also include instructions for using selected versions of commercial interfaces. The instructions are designed so that students can maximize the time spent understanding the ideas and the capabilities discussed in the book.

Answers to selected exercises are provided on the web site.

The software used for the exercises is freely available, open source, well documented, and widely used. The groundwater flow system is simulated using the Ground-Water Flow Process of MODFLOW-2000 (Harbaugh et al., 2000; Hill et al., 2000). The sensitivity analysis, calibration, and uncertainty aspects of the exercises can be accomplished using MODFLOW-2000's Observation, Sensitivity, and Parameter-Estimation Processes or UCODE_2005 (Poeter et al., 2005). Most of the sensitivity analysis, calibration, and uncertainty aspects of the exercises also can be conducted using PEST (Doherty, 1994, 2005). Relevant capabilities of MODFLOW-2000 and UCODE_2005 are noted as methods and guidelines are presented; relevant capabilities of PEST are noted in some cases. The public-domain programs for interface and visualization are MFI2K (Harbaugh, 2002), GWChart (Winston, 2000), and ModelViewer (Hsieh and Winston, 2002). The web sites from which these programs can be downloaded are listed with the references and on the book web site listed above.

The methods and guidelines presented in this book are broadly applicable. Throughout the book they are presented in the context of the capabilities of the computer codes mentioned above to provide concrete examples and encourage use.

PowerPoint files designed for teaching of the material in the book are provided on the web site. The authors invite those who use the PowerPoint files to share their additions and changes with others, in the same spirit with which we share these files with you.

The use of trade, firm, or product names in this book is for descriptive purposes only and does not imply endorsement by the U.S. Government.

The rest of this introductory chapter provides a brief overview of how regression methods fit into model calibration (Section 1.2), some perspective of how the ideas presented here relate to other ideas and past work (Section 1.3), some definitions (Section 1.4), a description of expertise that would assist readers and how to obtain that expertise (Section 1.5), and an overview of Chapters 2 through 15 (Section 1.6).

1.2 MODEL CALIBRATION WITH INVERSE MODELING

During calibration, model input such as system geometry and properties, initial and boundary conditions, and stresses are changed so that the model output matches related measured values. Many of the model inputs that are changed can be characterized using what are called "parameters" in this work. The measured values related to model outputs often are called "observations" or "observed values," which are equivalent terms and are used interchangeably in this book.

The basic steps of model calibration are shown in Figure 1.1. In the context of the entire modeling process, effectively using system information and observations to constrain the model is likely to produce a model that more accurately represents the simulated system and produces more accurate predictions, compared to a modeling procedure that uses these types of data less effectively. The ideas, methods, and guidelines presented in this book are aimed at helping to achieve more effective use of data.

The difficulties faced in simulating natural systems are demonstrated by the complex variability shown in Figure 1.2 as discussed by Zhang et al. (2006).

Four issues fundamental to model calibration are discussed in the next four sections. These include parameter definition or parameterization, which is the mechanism used to obtain a tractable and hopefully meaningful representation of

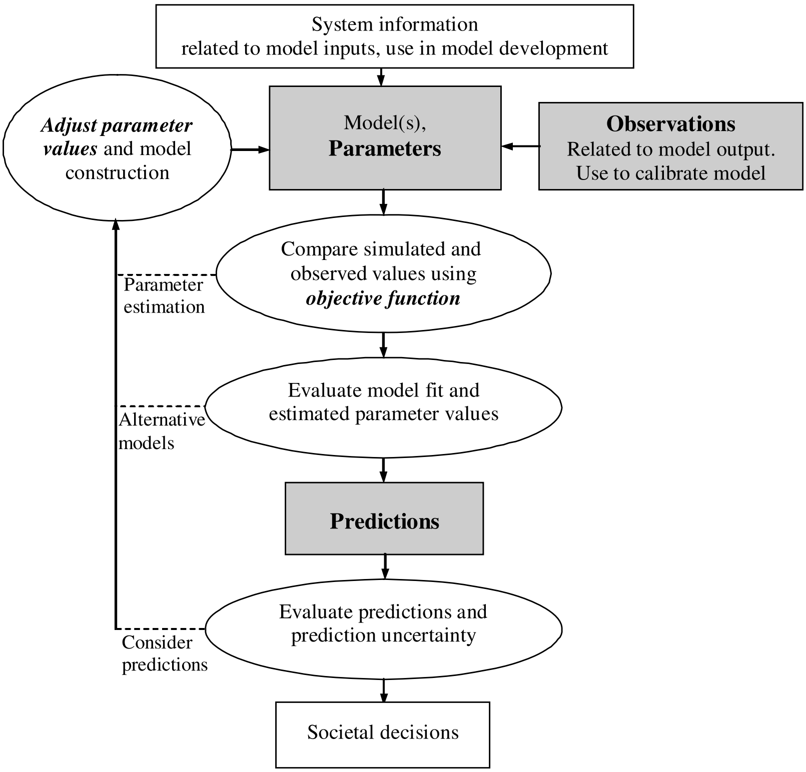

FIGURE 1.1 Flowchart showing the major steps of calibrating a model and using it to make predictions. Bold, italicized terms indicate the steps that are directly affected by nonlinear regression, including the use of an objective function to quantify the comparison between simulated and observed values. Predictions can be used during calibration as described in Chapter 8. (Adapted from Herb Buxton, U.S. Geological Survey, written communication, 1990.)

FIGURE 1.2 Experimental results from a subsiding tank, showing the kind of complexity characteristic of deltaic deposits in a subsiding basin. (Reproduced with permission from Paola et al. 2001.)

systems such as that shown in Figure 1.2; the objective function mentioned in Figure 1.1; the utility of inverse modeling, which is also called parameter estimation in this book; and using the model to quantitatively connect observations, parameters, and predictions.

1.2.1 Parameterization

The model inputs that need to be estimated are often distributed spatially and/or temporally, so that the number of parameter values could be infinite. The observations, however, generally are limited in number and support the estimation of relatively few parameters. Addressing this discrepancy is one of the greatest challenges faced by modelers in many fields. Typically, so-called parameterization is introduced that allows a limited number of parameter values to define model inputs throughout the spatial domain and time of interest. In this book, the term "parameter" is reserved for the values used to define model inputs. Consider the parameters defined in three groundwater model examples.

Example 1: One parameter represents the hydraulic conductivity of a hydrogeologic unit that occupies a prescribed volume of the model domain and is hydraulically distinctive and relatively uniform.

Example 2: One parameter represents a scalar multiplier of spatially varying recharge rates initially specified by the modeler for a given geographic area on the basis of precipitation, vegetation, elevation, and topography.

Example 3: One parameter represents the hydraulic head at a constant-head boundary that is used to simulate the water level in a lake.

This book focuses primarily on models for which a limited number of parameters are defined. Alternative methods are discussed in Section 1.3.2.

Historically, observed and simulated values, such as hydraulic heads, flows, and concentrations for groundwater systems, often were compared subjectively, so that it was difficult to determine how well one model was calibrated relative to another. In addition, in modeling of groundwater and other types of systems, adjustments of parameter values and other model characteristics were accomplished mostly by trial and error, which is time consuming, subjective, and inconclusive.

Formal methods have been developed that attempt to estimate parameter values given a mathematical model of system processes and a set of relevant observations. These are called inverse methods, and generally they are limited to the estimation of parameters as defined above. Thus, the terms "inverse modeling" and "parameter estimation" commonly are synonymous, as in this book. For some models, the inverse problem is linear, in that the observed quantities are linear functions of the parameters. In many circumstances of practical interest, however, the inverse problem is nonlinear, and its solution is not as straightforward as for linear problems. This book discusses methods for nonlinear inverse problems. One method of solving such problems is nonlinear regression, which is the primary solution method discussed in this book.

The complexity of many real systems and the scarcity of available data sets result in inversions that are often plagued by problems of insensitivity, nonuniqueness, and instability, regardless of how model calibration is achieved. Insensitivity occurs when the observations do not contain enough information to support estimation of the parameters. Nonuniqueness occurs when different combinations of parameter values match the observations equally well. Instability occurs when slight changes in, for example, parameter values or observations radically change simulated results. All these problems are exacerbated when the system is nonlinear. These problems are usually more easily detected when using formal inverse modeling and associated methods than when using trial-and-error methods for calibration. Detecting these problems is important to understanding the value of the resulting model.

1.2.2 Objective Function

In inverse modeling, the comparison of simulated and observed values is accomplished quantitatively using an objective function (Figure 1.1). The simulated and observed values include system-dependent variables (e.g., hydraulic head for the groundwater flow equation or concentration for the groundwater transport equation) and other system characteristics as represented by prior information on parameters. Parameter values that produce the "best fit" are defined as those that produce the smallest value of the objective function.

1.2.3 Utility of Inverse Modeling and Associated Methods

Recent work has clearly demonstrated that inverse modeling and associated sensitivity analysis, data needs assessment, and uncertainty evaluation methods provide capabilities that help modelers take greater advantage of their models and data, even for simulated systems that are very complex (i.e., Poeter and Hill, 1997; Faunt et al., 2004). The benefits include

1. Clear determination of parameter values that produce the best possible fit to the available observations.
2. Graphical analyses and diagnostic statistics that quantify the quality of calibration and data shortcomings and needs, including analyses of model fit, model bias, parameter estimates, and model predictions.
3. Inferential statistics that quantify the reliability of parameter estimates and predictions.
4. Other evaluations of uncertainty, including deterministic and Monte Carlo methods.
5. Identification of issues that are easily overlooked when calibration is conducted using trial and error methods alone.

Quantifying the quality of calibration, data shortcomings and needs, and uncertainty of parameter estimates and predictions is important to model defensibility and transparency and to communicating the results of modeling studies to managers, regulators, lawyers, concerned citizens, and to the modelers themselves.

Despite its apparent utility, in many fields, such as groundwater hydrology, the methods described in this book are not routinely used, and calibration using only trial-and-error methods is more common. This, in part, is due to lack of familiarity with the methods and the perception that they require more time than trial-and-error methods. It is also because inverse modeling and related sensitivity analysis methods clearly reveal problems such as insensitivity and nonuniqueness, and thereby reveal inconvenient model weaknesses. Yet if they are revealed, such weaknesses often can be reduced or eliminated. This occurs because knowledge of the weaknesses can be used to determine data collection and model development effort needed to strengthen the model. We hope this text will encourage modelers to use, and resource managers to demand, the more transparent and defensible models that result from using the types of methods and ideas described in this book.

1.2.4 Using the Model to Quantitatively Connect Parameters, Observations, and Predictions

The model quantitatively connects the system information and the observations to the predictions and their uncertainty. The entities Parameters, Observations, and Predictions are in bold type in Figure 1.1 because these entities are directly used by or produced by the model, whereas the system information often is indirectly used to create model input. Many of the methods presented in this book take advantage of the quantitative links the model provides between what is referred to in this book as the triad of the observations, parameters, and predictions.

The depiction of model calibration shown in Figure 1.1 is unusual in that it suggests simulating predictions and prediction uncertainty as model calibration proceeds. When execution times allow, it is often useful to include predictive analyses during model calibration so that the dynamics affecting model predictions can be better understood. Care must be taken, of course, not to use such simulations to bias model predictions.

1.3 RELATION OF THIS BOOK TO OTHER IDEAS AND PREVIOUS WORKS

This section relates the ideas of this book to predictive models and other literature.

1.3.1 Predictive Versus Calibrated Models

When simulating natural systems, the objective is often to produce a model that can predict, accurately enough to be useful, for assessing the consequences of introducing something new in the system. In groundwater systems, this may entail new pumpage or transport of recently introduced or potential contamination.

Ideally, model inputs would be determined accurately and completely enough from directly related field data to produce useful model results. This is advantageous because the resulting model is likely to be able to predict results in a wide range of circumstances, and for this reason such models are called *predictive models* (e.g., see Wilcock and Iverson, 2003; National Research Council, 2002). However, commonly quantities simulated by the model can be more readily measured than model inputs. The best possible determination of model inputs based on directly related field data can produce model outputs that match the measured equivalents poorly. If the fit is poor enough that the utility of model predictions is questionable, then a decision needs to be made about how to proceed. The choices are to use the predictive model, which has been shown to perform poorly in the circumstances for which testing is possible, or to modify the model so that, at the very least, it matches the available measured equivalents of model results. A model modified in this way is called a *calibrated model*.

There is significant and important debate about the utility of predictive and calibrated models, and it is our hope that the debate will lead to better methods of measuring quantities directly related to model inputs. We would rejoice with all others in the natural sciences to be able to always use predictive models. Until then, however, it is our opinion that methods and guidelines that promote the best possible use of models and data in the development of calibrated models are critical. It is also our belief that such methods and guidelines can play a role in informing and focusing the efforts of developing field methods that may ultimately allow predictive models to be used in more circumstances.

1.3.2 Previous Work

For the most part, comments in this introductory chapter are limited to the history, evolution, and status of nonlinear regression and modeling as related to groundwater systems. Comments about how specific methods or ideas relate to previous publications appear elsewhere in the book. This section contains the broadest discussion of parameterization methods presented in the book.

The topics covered by this book have been addressed by others using a variety of different methods, and have been developed for and applied to many different fields of science and engineering. We do not attempt to provide a full review of all work on these topics. Selected textbooks are as follows. Parker (1994), Sun (1994), Lebbe (1999), and Aster et al. (2005) discuss nonlinear regression in the field of geophysics. More general references for nonlinear regression and associated analyses include Bard (1974), Beck and Arnold (1977), Belsley et al. (1980), Seber and Wild (1989), Dennis and Schnabel (1996), and Tarantola (2005). Saltelli et al. (2000, 2004) provide comprehensive overviews of sensitivity-analysis methods. This book focuses on what Saltelli et al. describe as local sensitivity methods, and includes new sensitivity-analysis methods not included in the previous books.

The pioneers of using regression methods in groundwater modeling were Cooley (1977) and Yeh and Yoon (1981). Some of the material in this book was first published in U.S. Geological Survey reports (Cooley and Naff, 1990; Hill, 1992; Hill, 1994; Hill, 1998). Cooley and Naff (1990) presented a modified Gauss–Newton method of nonlinear regression that with some modification is used in Chapter 5, and residual analysis ideas derived from early editions of Draper and Smith (1998) that are used in Chapter 6. Hill (1992) presents sensitivity-analysis and residual-analysis methods used in Chapters 4 and 6. Cooley and Naff (1990), and Hill (1992), and Hill (1994) present methods of residual analysis and linear uncertainty analysis that are used in Chapters 6 and 8. Hill (1998) enhanced the methods presented in the previous works and presents the first version of the guidelines that are described in Chapters 10 through 14. Various aspects of the guidelines have a long history, and relevant references are cited in later chapters. To the authors' knowledge, these guidelines provide a more comprehensive foundation for the calibration and use of models of complex systems than any similar set of published guidelines. In general, the book expands the previously presented material, presents some new methods, and includes an extensive set of exercises.

Achieving Tractable Problems Regression is a powerful tool for using data to test hypothesized physical relations and to calibrate models in many fields (Seber and Wild, 1989; Draper and Smith, 1998). Despite its introduction into the groundwater literature in the 1970s (reviewed by McLaughlin and Townley, 1996), regression is only starting to be used with any regularity to develop numerical models of complicated groundwater systems. The scarcity of data, nonlinearity of the regression, and complexity of the physical systems cause substantial difficulties. Obtaining tractable models that represent the true system well enough to yield useful results is arguably the most important problem in the field. The only options are (1) improving the data, (2) ignoring the nonlinearity, and/or (3) carefully ignoring some of the system complexity. Scarcity of data is a perpetual problem not likely to be alleviated at most field sites despite recent impressive advances in geophysical data collection and analysis (e.g., Eppstein and Dougherty, 1996; Hyndman and Gorelick, 1996; Lebbe, 1999; Dam and Christensen, 2003). Methods that ignore nonlinearity are presented by, for example, Kitanidis (1997) and Sun (1994, p. 182). The large changes in parameter values that occur in most nonlinear regressions of many problems after the first iteration, however, indicate that linearized methods are unlikely to produce satisfactory results in many circumstances. This leaves option 3, which is discussed in the following paragraphs.

Defining a tractable and useful level of parameterization for groundwater inverse problems has been an intensely sought goal, focused mostly on the representation of hydraulic conductivity or transmissivity. Suggested approaches vary considerably. The most complex parameterizations are cell- or pixel-based methods in which hydraulic conductivity or transmissivity parameters are defined for each model cell, element, or other basic model entity, and prior information or regularization is used to stabilize the solution (e.g., see Tikhonov and Arsenin, 1977; Clifton and Neuman, 1982; Backus, 1988; McLaughlin and Townley, 1996). The simplest parameterizations require homogeneity, such that, at the extreme, one parameter specifies hydraulic conductivity throughout the model.

As more parameters are defined and the information contained in the observations is overwhelmed, prior information on parameters and/or regularization on observations and/or parameters become necessary to attain a tractable problem. In this book, we use definitions of prior information and regularization derived from Backus (1988). When applied to parameters, prior information and regularization produce similar penalty-function terms in the objective function. For prior information, the weighting used approximates the reliability of the prior information based on either classical or Bayesian statistical arguments. Essentially, classical statistical arguments are based on sampling methods; Bayesian statistical arguments are, at least in part, based on belief (Bolstad, 2004). In contrast, for regularization the weighting generally is determined as required to produce a tractable problem, as represented by a unique set of estimated parameter values. The resulting weights generally are much larger than can be justified based on what could possibly be known or theorized about the parameter values and distribution. For both prior information and regularization, the values used in the penalty function need to be unbiased (see the definition in Section 1.4.2).

Between the two extreme parameterizations mentioned previously, there is a wide array of designs ranging from interpolation methods such as pilot points (RamaRoa et al., 1995; Doherty, 2003; Moore and Doherty, 2005, 2006) to zones of constant value designed using geologic information (see Chapter 15 for examples). For example, the Regularization Capability of the computer code PEST (Doherty, 1994, 2005) typically allows many parameters to be estimated. Indeed, the number of parameters may exceed the number of observations. Parameter estimation is made possible by requiring that the parameter values satisfy additional considerations. Most commonly, the parameter distribution is required to be smooth. This and other considerations are discussed by Tikhonov and Arsenin (1977) and Menke (1989). More recent approaches include the superparameters of Tonkin and Doherty (2006) and the representer method of Valstar et al. (2004). The former uses singular value decomposition to identify a few major eigenvectors from sensitivity matrices; only the "superparameters" defined by the eigenvectors are estimated by regression.