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Vikenti Gorokhovski

Effective Parameters of Hydrogeological Models

Second Edition

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Dedicated to my wife
Inna Gorokhovskaia

and

to the memory of our son
Iaroslav Gorokhovski
(1963–2011)

Preface to Second Edition

The main change made in this edition is a new chapter, Chap. 10, located between Chaps. 9 and 10 of the previous edition. It presents the method based on simulation of advective solute transport through porous media with direct inclusion of hydrodynamic dispersion. The method reduces solute transport simulation to solving partial differential equations of the first order for different actual pore water velocities which makes it very flexible. The ways of evaluating the actual pore water velocities are suggested also. The method is an alternative to the classical convective-dispersion model with it fictitious dispersion coefficient and the mean actual pore velocity, excluding hydraulic dispersion, the main reason for appearance of long tails of the observed breakthrough curves.

The history of this chapter appearance is following. A known hydrogeologist stated to Dr. Steven Kraemer, my supervisor at that time, that the use of the first type boundary condition in simulation of solute transport in porous media is incorrect. He suggested overwriting all related software used by Environmental Protection Agency, U.S.A., applying the boundary condition of the third type, the flux condition, the only correct boundary condition, according to him. Before discussing the issue with his supervisors, Steve asked me to clarify the situation. The most detail basis for introducing the flux boundary condition which I could find is the work of Parker and van Genuchten (1984). In my opinion the basis was unsatisfactory, doubtful mathematically and physically, which I reported to Steve. After becoming a free lance hydrogeologist, I got more free time and took part in discussion (Gorokhovski 2013) on Batu (2010) holding that the flux condition is the only correct one because it keeps mass-balance at the inlet. In the response to my criticism, (Batu et al. 2013) do not refute my arguments but continue insist that the flux boundary condition is the only correct one. It is obvious that the use of the mean pore velocity in the classical model eliminates hydraulic dispersion from it. The empirical dispersion coefficient should, as if, compensate for the hydraulic dispersion. How this fictitious coefficient does the job was never explained, and it does not factually. Long tails of the observed breakthrough curves exists due mostly hydraulic dispersion. The impossibility in most cases to reproduce them by simulation breakthrough curves is clear demonstration of this. The issue of fitting the simulation breakthrough curves into the observed long tailed ones was the main motivation for Parker and van Genuchten (1984) to introduce the flux boundary condition. Likely, its application did not resolve the issue (Parker and van Genuchten 1984; Paseka et al. 2000; Delleur 2006; Dušek et al. 2007; Appuhamillage et al. 2010).

Other changes include reviews of some works appeared after publishing of the first edition of this book or related to Chap. 10. Thus, in distinction from the previous edition, all examples related to solute transport are concentrated in this chapter to minimize the necessary changes in the book. Few misprints and inaccuracies slipped into the previous text were corrected also.

Acknowledgments

I would like to express my gratitude to Dr. Steven Kraemer, my friend and one of my supervisors, without whose suggestion to clear up the issue with the flux boundary condition in solute transport simulation this edition would never happen. As usual, my wife Inna and our son Vikenti were supportive and extremely helpful in my work.

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Preface to the First Edition

This book concerns the uncertainty of the hydrogeological modeling. In a sense, it is a development of the ideas published long ago (Gorokhovski 1977). The topic of that book was impossibility of evaluating the uncertainty of the simulation results in a provable quantitative way. The book happened to be a success: I had difficulty finding its copies for my friends, some prominent hydrogeologists and geological engineers started treating me with more respect, and some colleagues stopped speaking to me for a long time. But no other consequences followed.

I personally was not fully satisfied. The book was mostly a critique based on common sense and illustrated by simple and transparent examples from hydrogeology and geological engineering. The examples could be easily verified, using just a calculator. The book stated that the impossibility to evaluate the uncertainty of simulation results does not preclude obtaining the results which are best in a reasonably defined sense, though the uncertainty of those best results remains unknown. But I had a vague notion on how to assure such results at that time.

Quantitative predictions of responses of geological objects on man made and natural impacts were, are, and will remain in the foreseeable future a considerable element of engineering design and decision making. Even in that time and even in the Soviet Union, where I resided and worked, it was possible to simulate many applied hydrogeological processes, though access to the pertinent software and computers was not easy, at least for me (see Afterword for more details). At present, due to the fast development of computers and numerical methods, we can simulate almost any process based on contemporary concepts and theories. The gravest obstacle remains uncertainty of the simulation results caused by paucity of the available data on properties of geological objects, boundary conditions, and impacts when the natural impacts are affecting factors. So one of the main issues, in my opinion, is how to assure that the yielded results are the best, effective, in the sense as the best is defined. I hope that this book is a considerable step to yielding the effective simulation results.

The uncertainty of the results of hydrogeological modeling was and is discussed intensively. Thus, Beck (1987) writes: “The difficulties of mathematical modeling are not questions of whether the equations can be solved and the cost of solving them many times; not are they essentially questions of whether priory theories (on transport, dispersion, growth, decay, predation, etc.) is potentially capable of describing the system’s behavior. The important questions are those whether the priory theory adequately matches observed behavior and whether the predictions obtained from models are meaningful and useful". Oreskes et al. (1994) hold that geological models "predictive value is always open to question". (See also, Oreskes 2003, 2004). This is not surprising, since in hydrogeology "the modeling assumptions are generally false and known to be false" (Morton 1993, Beven 2005). I could continue this list of similar quotations. But let me restrict myself with one more. As Beven (2004), puts it mildly: "There is uncertainty about uncertainty". I think he is wrong: the uncertainty of the hydrogeological modeling is the fact about which there is no uncertainty. Indeed: "It's a fundamental tenet of philosophy of science that the truth of a model can never be proved; only disproved," (Mesterton-Gibbons 1989).

The above quotations are a tribute to academism really. Experienced hydrogeologists are well aware of the uncertainty of most their conclusions. And the reason is obvious. The models include properties and combinations of the properties of geological objects. Those must be known continuously, at least, when differential or integral equations are involved. That is, they must be known at each point of the object and at each instant of the simulation period, excluding sets of isolated points and instants. But geological objects are inaccessible to direct observations and measurements and the data on them are sparse. The geological models are a tool to interpolate and extrapolate the sparse data at every point of the geological object which they represent in simulations and at very instant of the periods of the simulations. The tool is limited. The geological interpolation and extrapolation are based on the principle that geological settings of the same origin, composition, and geological history have the same properties. This principle leads to so-called piecewise homogeneous geological models. Sometimes, the properties are subjected to spatial trends whose mathematical descriptions are arbitrary in essence (Chap. 3). So how can we evaluate in a quantitative way the reliability of the geological models with respect to a problem at hand? It suffices just a common sense to conclude that it is impossible except, maybe, in some rare cases.

Since the issue is not simulations, solving the corresponding equations, but the uncertainty of the yielded results, the question arises, what to do? U.S. EPA (1987) gives the answer related to environmental predictions, including hydrogeological ones: "It should be recognized that the data base will always be inadequate, and eventually there will be a finite sum that is dictated by time, common sense, and budgetary constraints. One simply has to do the best one can with what is available". Unfortunately, (U.S. EPA, 1987) does not explain what is and how to do "the best".

The situation seems to be clear enough: it is impossible to evaluate the uncertainty of simulation results of the hydrogeological models in a provable quantitative way. But, contrary to its own statement cited above U.S. EPA (1989) holds that "Sensitivity and uncertainty analysis of environmental models and their predictions should be performed to provide decision -makers an understanding of the level of confidence in model results and to identify key areas for future study". It claims also that "A number of methods have been developed in recent years for quantifying and interpreting the sensitivity and uncertainty of models". NCR

(1990) states “Over the past decade, the development of stochastic modeling techniques has been useful in quantitatively establishing the extent to which uncertainty in model input translates to uncertainty in model prediction”. Binley and Beven (1992), Beven and Freer (2001) and Beven (2005), suggest a general likelihood framework for uncertainty analysis, recognizing that it includes some subjective elements and, therefore, in my opinion, may not be provable. Hill et al. 2000, suggest the algorithm and program, permitting evaluating the uncertainty of simulation results. Cooley, 2004, suggests a theory for making predictions and estimating their uncertainty. And so on (Feyen and Caers 2006; Hassan et al. 2008; Rojas et al. 2008, 2010; Ch and Mathur 2010; Mathon et al. 2010; Ni el at. 2010; Singh et al. 2010a, b; Zhang et al. 2010; Doherty and Christensen 2011, and others).

For example, Doherty and Christensen (2011) hold in the abstract to their paper that it “describes a methodology for paired model usage through which predictive bias of a simplified model can be detected and corrected, and postcalibration predictive uncertainty can be quantified”. However, they write closer to the end of their paper: “In designing and implementing the methodology discussed herein, we have assumed that the processes and construction details of the complex model approximate those of reality. It is obvious that this will not always be the case. Indeed, even the most complex model is quite simple compared to reality itself. In spite of this, a modeler can only do his or her best”. Something like this has been already quoted (EPA, 1987). But let us continue. Several lines below their previous statement Doherty and Christensen (2011) write: “Nevertheless, the less than perfect nature of a complex model, and its consequential failure to represent all nuances of system behavior, may indeed result in some degree of underestimation of predictive uncertainty. This, unfortunately, is unavoidable”.

I pay more attention to the work of Doherty and Christensen (2011) not only because it is one of the most recent ones on the uncertainty of hydrogeological simulation, but because it is typical. Many, if not most, of such publications proclaim in the very beginning that a method of quantifying of the simulation uncertainty is being suggested. However, somewhere closer to the end, the authors explain that they can estimate the uncertainty to some degree. The authors, being excellent mathematicians, understand that their simulations are based on a number of explicit and implicit assumption, hypotheses, and simplifications most of which cannot be validated or are knowingly false. So their estimates of the uncertainty are not provable. This is from where all these “to some degree” appear. The Polish poet and aphorist Jerzy Lec told about such kind of situations: “Impolitely to speak ‘it seems’ when everything is already clear”.

Doherty and Christensen (2011) attracted my attention also because their methodology of the paired model usage, at first glance, seems to be similar to the two-level modeling described in this book and presented previously, in various contexts related to its different possible use (Gorokhovski 1986, 1991, 1996, 2012; Gorokhovski and Konivetski 1994; Gorokhovski and Nute 1995, 1996). While seemingly alike, the paired model usage and the two-level modeling differ with respect to their mathematics and goals. The goal, as well as mathematics, of the two-level modeling is much more modest: It recognizes the impossibility to quantify the uncertainty of simulation results in a provable way and is focused just on obtaining the best simulation results in reasonably predefined senses.

Although the number of publications providing the methods, as if, quantifying uncertainty of the results of hydrogeological modeling growths very fast, they cannot call off the philosophical tenet which leaves us still with the only real option: "to do the best one can with what is available". In this book, it means obtaining the best simulation results in the sense of the least squares criterion on a given monitoring network, though other criteria of the efficiency are possible also. Besides, the required 'the best' must relate not to the best fit during model identifications (calibrations), but to the best results in the coupled predictive simulations. Such simulation results are called effective. To achieve the predictive efficiency for a given simulation model, we need to find the effective parameters, that is, the parameters making the pertinent predicting or evaluating effective. A model furnished with the effective parameters is called effective. Once more, the goal must be the models which are effective in predictive simulations and extended evaluations, not in model identification procedures like calibration. This can be achieved by introducing the transforming mechanisms converting the actual properties of geological bodies into effective parameters of the predictive models (Chap. 5). Chapters 6 and 7 contain examples of such mechanisms. The standard procedure for evaluating the transforming mechanisms is called by me the two-level modeling (Chap. 8). The transforming mechanisms can be applied for solving inverse problems (Chap. 9). The notion of the inverse problem in this book differs from the standard one accepted in hydrogeological modeling. That is, the inverse problem is understood as evaluating properties of more complex models using less complex ones. This second edition contains new Chap. 10 discussing solute transport through porous media. Chap. 11 is a short conclusion. The book ends with Chap. 12 in which I compare my Soviet and American experiences as a teacher and a scientist. I hope it may by interesting for readers.

I hope that this book can be helpful for modelers working with the underground flows and mass transport. But its main addressees are common hydrogeologists and, maybe, students of hydrogeology and environmental sciences. I knew and know many excellent hydrogeologists who never differentiated or integrated anything after passing the final tests on calculus. For these reasons, I resort to the sound sense and the simplest mathematical models and examples, rather of the conceptual nature, i.e., "constructed to elucidate delicate and difficult points of a theory" (Lin and Segel 1974, Kac 1969) as much as I can. However, the approach to alleviating the issue of the uncertainty of the results of hydrogeological simulations suggested in this book requires intensive computational calculations. This does not permit avoiding mathematics completely. But the mathematics applied in the text is mostly the least squares method. The examples and the results are transparent and easy to understand and to interpret even for those readers who do not want to mess with mathematics.

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This book would not be possible without help of many people from different walks. Among them I have to mention first experienced hydrogeologist and dear friend L. S. Yazvin, who passed away recently. Our uncompromised disputes have done a lot to form my approaches to hydrogeological modeling. Fair criticism and support of my friends and colleagues, B. V. Borevsky, M. T. Oyzerman, M. V. Rats, and V. V. Trofimov helped me in the development of the two-level modeling approach. I cannot but mention V. I. Sedletsky without whom the probability of my coming to the United States and writing this book had been extremely low. This book would be impossible without Dr. Zia Hosseinipour who found a project for me in this country and helped, as well as our dear friends Mr. and Mrs. Donald and Karen Goodel, to get and to settle me and my wife here. I thank and value my American supervisors, Drs. James Martin, Donald Nute, Dan Kannan, and Jim Weaver who became my friends. They were kind to let me apply my strange approaches to the problems they assigned to me. I thank my sons Vikenti and Iaroslav for their support and help. And of course, this endeavor would be impossible without support, help and endurance of my beloved wife Inna.

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Contents

Abstract

Geological models applied to predictive hydrogeological modeling are not exact replicas of the objects they represent. Manifold details related to structures and properties of the objects remain unknown. Those details can affect simulation results considerably, differently, and unpredictably for different formulations of the simulation problem. They cause the phenomenon of problem-dependence of model identification, make the model parameters, effective in calibration, ineffective in predictive simulations and do not permit the provable evaluation of uncertainty of the simulation results. However, this does not preclude obtaining the best, effective, simulation results based on the available data and predefined criteria of quality of predicting. To provide such results, transforming mechanisms are introduced. They are mathematical expressions for evaluating the model parameters, which are effective in predictive simulations. Examples of the mechanisms are provided as well as method of their evaluation, and how the mechanisms can be used for interpretation hydrogeological data is also shown. In this edition, a new chapter is included suggesting, as alternative to the dispersive-convective model of solute transport through porous media, the advective model taking in consideration hydraulic dispersion and demonstration of its advantage. In his last chapter, the author compares the conditions under which he worked in the Soviet Union (35 years) and in the United States (20 years) which may be interesting for readers.

Chapter 1
Introduction

Although hydrogeological conditions can be of interest per se, most of hydrogeological investigations are of applied nature, and their results are used in decision-making that may carry large ecological and financial risks. For example, when developing a reservoir project, the developers have to evaluate possible losses of water from the reservoir, stability of the dam and how the adjacent soils and rocks could be affected by different project decisions. Hydrogeological investigations related to the use of an aquifer for water supply should not only conclude that the usage is possible. The developers must also have estimates on how long and with what intensity the aquifer can be exploited by a well or a group of wells. The developers of a landfill project must know whether the landfill can cause contamination of the aquifer below and, if so, whether and when the contaminant plume reaches water supply wells and the concentration of the pollutant at the wells. The developers of an irrigation project need to know to what extent and how fast the water table rise should be expected, what consequences are possible and how to deal with them, etc.

The point is that for the projects that affect geological surroundings to be effective environmentally and economically, the responses of the surroundings to the planning impacts must be taken in consideration. To this end the goal of the applied hydrogeological investigations is to provide quantitative predictions of those responses. Moreover, to make a correct or optimal decision, decision-makers must know the errors of the quantitative predictions. (The term ‘to predict’ relates to the processes developing in time. In this text it is used also as a synonyms of the term ‘to evaluate’ in cases of evaluating some instant value or steady state conditions, if such usage does not cause confusion.)

The usual tool for obtaining quantitative hydrogeological predictions is mathematical modeling, i.e., solving differential and integral equations describing the pertinent processes or states. The mathematical models are applied to the geological models substituting for real geological objects. In this book, the mathematical models are assumed to be adequate, i.e., that they reproduce the processes of interest sufficiently accurately. This is not true in general (see Chap. 10), but the mathematical models recognized by the professional community and applied properly usually yield satisfying approximations of the reality. The main source of

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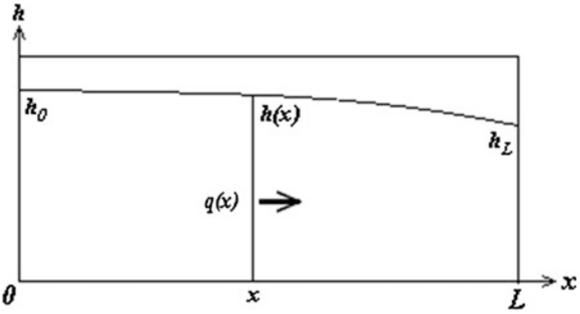
Fig. 1.1 One-dimensional steady state flow on interval [0, *L*]



the errors occurring in simulations is the distinction between predictive geological models and actual geological objects, and inaccurate or often just wrong boundary conditions, though inaccuracies of the mathematical models also contribute in those errors. Since the geological surroundings are inaccessible to direct observations and measurements, and data on them are sparse, the issue is how the parts of geological objects which are unknown or wrongly presented by geological models can affect the accuracy of the simulation results.

Let us start with simple example: steady-state filtration in an unconfined aquifer on a horizontal base when the recharge is absent (Fig. 1.1). Under the Dupuit-Forchheimer assumption (simplification), considering the vertical component of the Darcy velocity to be negligibly small, the filtration can be treated as one-dimensional. It is governed by the following ordinary differential equation

$$\frac{d\left(K(x)h(x)\frac{dh}{dx}\right)}{dx} = 0 \tag{1.1}$$

where $h(x)$ is the thickness of the aquifer at point x and $K(x)$ is the hydraulic conductivity varying along the x-axis. Equation 1.1 is derived based on the law of conservation and the Darcy law stating that the velocity of filtration q (the Darcy velocity, specific flux) is equal to

$$q = -K(x)\frac{dh}{dx}. \tag{1.2}$$

The boundary conditions are the thickness of the aquifer at the ends of interval [0, L] which is assumed to be known: $h(0) = h_0$ and $h(L) = h_L$.

Let the goal be to evaluate the thickness of the aquifer at any arbitrary location x within interval [0, L]. To this end, we have to integrate Eq. 1.1. Its first integration yields

$$2K(x)h(x)\frac{dh}{dx} = C$$