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Vikenti Gorokhovski

Effective Parameters of Hydrogeological Models

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Dedicated to my wife
Inna Gorokhovskaia
and to the memory of our son
Iaroslav Gorokhovski
(1963–2011)

Preface

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 of 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 at 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, and effective in the sense 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 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 of 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 every 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 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? US 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, US 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 (US EPA, 1989), holds that "Sensitivity and uncertainty analysis of environmental models and their predictions should be performed to provide decision-makers with 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 into 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 and Bekhit 2008; Rojas et al. 2008, 2010; Ch and Mathur 2010; Mathon et al. 2010; Ni et al. 2010; Singh et al. 2010a, b; Zhang et al. 2009; and many others).

Although the number of publications providing the methods as if quantifying uncertainty of the results hydrogeological modeling growths very fast, the philosophical tenet mentioned above 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 also possible. Besides, the required 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, and 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. Chapter 10 is a short conclusion. I included in the book Chap. 11 also where 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 is 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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Contents

Abstract

Effective Parameters of Hydrogeological Models Geological models applied in predictive hydrogeological modeling are not exact replicas of the objects they represent. Manifold of details related to structures and properties of the objects remains unknown. Those details affect the simulation results considerably, differently and unpredictably for different formulations of the simulation problem. They cause the phenomenon of problem-dependence of model identification and make the model parameters effective in calibration ineffective in predictive simulations. Due to them the provable evaluation of uncertainty of the simulation results is impossible. 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 a method for their evaluations. Shown also how the mechanisms can be used for interpretation hydrogeological data which is possible due to the mention above phenomenon of the problem-dependence. In his last chapter 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 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, the stability of the dam, and how 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 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 will reach 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, how to deal with them effectively, etc.

The point is that, for projects that affect the geological surroundings to be effective environmentally and economically, the responses of the surroundings to the planning impacts must be taken into consideration. To this end, the goal of 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 processes developing in time. In this text it is used also as a synonym for 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 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

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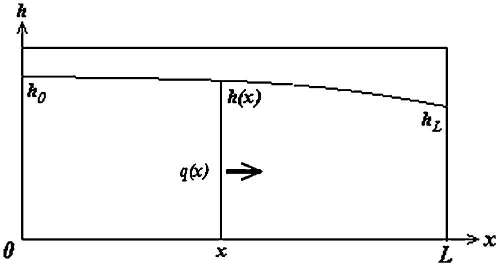

Fig. 1.1 One-dimensional steady-state flow on the interval [0, L]

interest sufficiently accurately. This is not true in general, but mathematical models recognized by the professional community and applied properly usually yield satisfactory approximations of reality (see Sect. 4.4). The main source of error 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 to 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 represented by geological models can affect the accuracy of the simulation results.

Let us start with a simple example: steady-state filtration in an unconfined aquifer on a horizontal base when recharge is absent (Fig. 1.1). Under the Dupuit–Forchheimer assumption, 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:

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

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

$$q = -K(x)\frac{\mathrm{d}h}{\mathrm{d}x}. \tag{1.2}$$

The boundary conditions are the thickness of the aquifer at the ends of the 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 the interval [0, L]. To this end, we have to integrate Eq. 1.1. Its first integration yields

$$2K(x)h(x)\frac{\mathrm{d}h}{\mathrm{d}x} = C,$$

where C is an arbitrary constant (the factor of 2 being used to simplify Eq. 1.3 below). Assuming that $K(x) \neq 0$ in the interval [0, L], we can rewrite the above equation as

$$2h(x)\mathrm{d}h = C\frac{\mathrm{d}x}{K(x)}.$$

Integrating the above equation, we obtain

$$2\int_0^x h(x)\mathrm{d}h = h^2(x) - h^2(0) = C\int_0^x \frac{\mathrm{d}x}{K(x)}. \qquad (1.3)$$

To obtain a unique solution to Eq. 1.1, we need to define the arbitrary constant C. To this end we use the second boundary condition at $x = L$:

$$h_L^2 = C\int_0^L \frac{\mathrm{d}x}{K(x)} + h_0^2 \text{ and } C = -\frac{h_0^2 - h_L^2}{\int_0^L \frac{\mathrm{d}x}{K(x)}}.$$

Then, the solution to Eq. 1.1 with the given boundary conditions takes the form

$$h^2(x) = h_0^2 - \left(h_0^2 - h_L^2\right)\frac{\int_0^x \frac{\mathrm{d}x}{K(x)}}{\int_0^L \frac{\mathrm{d}x}{K(x)}}. \qquad (1.4)$$

Thus, to obtain the thickness of the aquifer, $h(x)$, at an arbitrary point x within the interval [0, L], we need to know the boundary conditions h_0 and h_L at the ends of the interval and the hydraulic conductivity, $K(x)$, continuously, i.e. at each point of the interval, excluding perhaps a countable set of points (i.e., a set of points that can be enumerated, meaning separated from each other).

However, knowing $K(x)$ at each point of the interval of interest is not possible physically or economically. A few, sparse measurements of the hydraulic conductivity are available at best. We need to fill in the information gap by interpolating and extrapolating the available data on the hydraulic conductivity over all points of the interval [0, L]. Tools for doing this are geological (structural) models (which I prefer to call geological ones, to emphasize that geologists with their knowledge of geological settings and their spatial variability play the most important role in interpolating and extrapolating geological data). The tools are usually limited and even primitive. They are based on the principle that soils and rocks of the same origin, lithological composition, geological age, and history are homogeneous geologically; that is, each property of a geologically homogeneous structure is considered constant. Simple trends in the property values are permissible, if the data reveal some spatial tendencies. Model calibration is also a tool for generalization of the variable property values of interest in the predictive