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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.

Acknowledgements

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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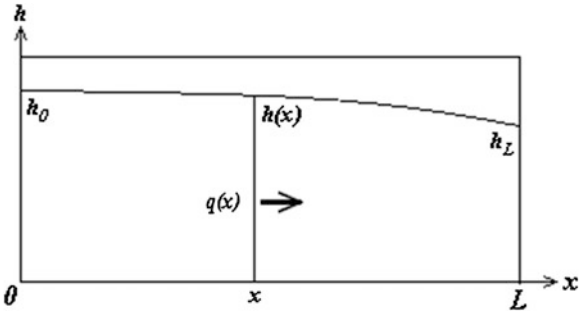

Fig. 1.1 One-dimensional steady state flow on interval [0, *L*]

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

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

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

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

Integrating the above equation, we obtain

$$2\int_0^x h(x)dh = h^2(x) - h^2(0) = C\int_0^x \frac{dx}{K(x)} \tag{1.3}$$

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 $x = L$:

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

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

$$h^2(x) = h_0^2 - \left(h_0^2 - h_L^2\right)\frac{\int_0^x \frac{dx}{K(x)}}{\int_0^L \frac{dx}{K(x)}} \tag{1.4}$$

Thus, to obtain the thickness of the aquifer, $h(x)$, at 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, maybe, a countable set of points (i.e., a set of points that can be enumerated, meaning separated from each other).

However, the knowledge of $K(x)$ at each point of the interval of interest is not possible physically and economically. A few, sparse measurements of the hydraulic conductivity are available at best. We need to fill the information gap by interpolating and extrapolating the available data on the hydraulic conductivity over all points of interval [0, L]. Tools for doing this are geological (structural) models (I prefer to call these models the geological ones, to emphasize that geologists with their knowledge of geological settings and their spatial variability play the most important part in interpolating and extrapolating geological data). The tools are usually limited and even primitive. They are based on the principle that the soils and rocks of the same origin, lithological composition, geological age and history are homogeneous geologically. That is, each property of 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 model parameters (see Chap. 4). Another approach to filling the information gap is the use of random functions as a tool for describing spatial

distributions of the geological properties (see Chap. 3). Both approaches can be combined: geologists assign boundaries of geologically homogeneous parts of a site, and different regressions and random functions can be used within those geologically homogeneous parts.

The simplest interpolation in the considered example is recognizing the aquifer as homogeneous within interval [0, L] with the constant hydraulic conductivity $K(x) = \hat{K}$. Then the constant hydraulic conductivity $\hat{K}$ can be factored out from Eq. 1.1 or 1.4 and canceled, converting Eq. 1.4 into

$$h^2(x) = h_0^2 - \left(h_0^2 - h_L^2\right)\frac{x}{L} \tag{1.5}$$

So as soon as the homogeneous model of the aquifer is chosen, the predicted aquifer thickness does not depend on the hydraulic conductivity at all. Since the actual hydraulic conductivity is not constant, the simulation results will carry errors. The only possible estimate for these errors is that the real water table elevations are between h_0 and h_L. The errors are equal to zero at the ends of interval [0, L] and reach the maximal absolute value somewhere inside the interval. The magnitude of the error does not exceed $|h_0 - h_L|$.

Let the previous scheme (Fig. 1.1) represent a cross section of a channel and a capturing drain, and the goal be to evaluate the losses, flux Q, from the channel to the drain parallel to the channel. The geological model is homogeneous still, though the geological object is not. The losses depend on the hydraulic conductivity of rocks and soils between the channel and the drain. Assuming the steady-state regime and absence of the infiltration within interval [0, L], we obtain the constant flux Q which is described by the following equation at arbitrary point x within interval [0, L]:

$$Q = -K(x)h(x)\frac{dh}{dx} \tag{1.6}$$

Separating variables, we can rewrite Eq. 1.6 as

$$Q\frac{dx}{K(x)} = -h(x)dh \tag{1.7}$$

Integrating Eq. 1.7 with the same boundary conditions ($h_0 = h(0)$ and $h_L = h(L)$), yields

$$Q = -\frac{h_0^2 - h_L^2}{2\int_0^L \frac{dx}{K(x)}} \tag{1.8}$$

In the case of the homogeneous model Eq. 1.8 yields

$$\hat{Q} = -\hat{K}\frac{h_0^2 - h_L^2}{2L} \tag{1.9}$$

So to evaluate the losses Q accurately, the effective hydraulic conductivity $\hat{K}$ of the homogeneous model must be assigned as

$$\frac{1}{\hat{K}} = \frac{1}{L}\int_0^L \frac{dx}{K(x)} \tag{1.10}$$

If the acceptable losses Q are known, and the soil between the canal and the drain can be compacted, Eq. 1.9 could be applied to evaluate the necessary degree of compression of the soil, but this is not the point here. Contrary to the case of evaluating thickness of the aquifer, applying the homogeneous model, in this case we are not able to evaluate the upper boundary for errors of the predicted losses Q, if we do not know the range of the actual values of the hydraulic conductivities $K(x)$. However, Eq. 1.10 gives the rule for assigning the hydraulic conductivity to the homogeneous models to estimate the losses, considering the Dupuit-Forchheimer assumption acceptable. It should be the *weighted harmonic mean* of the actual hydraulic conductivities.

The most popular geological models represent geological sites as consisting of homogeneous subintervals such that within subinterval $[x_{i-1}, x_i]$ the hydraulic conductivity is constant and equal to K_i. Then Eq. 1.10 can be rewritten as

$$\frac{1}{\hat{K}} = \frac{1}{L}\sum_{i=1}^{n}\left(\frac{1}{K_i}\int_{x_{i-1}}^{x_i} dx\right) = \frac{1}{L}\sum_{i=1}^{n}\frac{\Delta x_i}{K_i} \tag{1.11}$$

where n is the number of homogeneous subintervals and $\Delta x_i = x_i - x_{i-1}$. Thus, the hydraulic conductivity of the homogeneous model must be assigned as the harmonic mean weighted with respect to the length of the homogeneous subintervals. If the errors ΔK_i for the hydraulic conductivities K_i within each subinterval $[x_{i-1}, x_i]$ are known, evaluating the errors of the model parameter $\hat{K}$ and the losses of the flux Q becomes possible.

The above examples demonstrate that not only geological settings define the choice of model parameters, but also formulation of the simulation problem. Thus, when evaluating the thickness of the aquifer on the horizontal aquitard applying a homogeneous model under the Dupuit-Forchheimer simplification we do not need to worry about choosing the model hydraulic conductivity at all (rather avoid the homogeneous model in such sort of problems). However, evaluating the losses, we need to worry about assigning the model hydraulic conductivity. Moreover, as demonstrated in Chap. 6, the effective hydraulic conductivities (the model parameters providing the best fit of the simulation results to the observations) depend on the monitoring network. As shown in Chap. 7 the effective hydraulic transmissivities can depend on time also.

Gomez-Hernandez and Gorelick (1989), hold: "If there is no best effective hydraulic conductivity …, the predictive capability of the model must be questioned." Why? Two above examples are illustration of the well known

phenomenon called the problem-dependence of model identification (Gorokhovski 1977; Carrera and Neuman 1986; Yeh 1986; Kool et al. 1987; Hornung 1990; van Genuchten et al. 1990; Bear et al. 1992). The phenomenon does affect the predictive capability of the models. It means that the effective parameters of predictive model may be different for different formulations of the simulation problems. Namely, the issue of obtaining the model parameters which are effective in predictive simulations, not just in calibrations, is the main point of this book.

Let us consider two simple examples of assigning the hydraulic conductivity values to our homogeneous model according to Eq. 1.10 [more examples can be found in Gorokhovski (1977)]. In these examples, functions $K(x)$ are such that integral 1.10 can be found in any text-book on integral calculus.

First, let the hydraulic conductivity be a linear function of the coordinates:

$$K(x) = \frac{K_L - K_0}{L} x + K_0$$

where $K_0 = K(0)$ and $K_L = K(L)$. Then according to Eq. 1.10,

$$\frac{1}{\hat{K}} = \frac{1}{L} \int_0^L \frac{dx}{\frac{K_L - K_0}{L} x + K_0} = \frac{1}{K_L - K_0} \, ln \, \frac{K_L}{K_0}$$

Thus,

$$\hat{K} = \frac{K_L - K_0}{ln \frac{K_L}{K_0}} \tag{1.12}$$

Second, let the hydraulic conductivity be an exponential function:

$$K(x) = K_0 e^{-\frac{x}{L}} K(x) - K_0 e^{-\frac{x}{L}}$$

Substituting the above $K(x)$ into Eq. 1.10, we obtain

$$\frac{1}{\hat{K}} = \frac{1}{L} \int_0^L \frac{dx}{K_0 e^{-\frac{x}{L}}} = \frac{1}{K_0} \int_0^L e^{\frac{x}{L}} \frac{dx}{L} = \frac{1}{K_0} (e - 1)$$

So in this case

$$\hat{K} = \frac{K_0}{e - 1} \tag{1.13}$$

Equations 1.12 and 1.13 also represent the harmonic means of the actual values of hydraulic conductivities under their specific spatial distributions. What is important, is that no statistical or probabilistic concepts or notions are applied to yield those results. They have been obtained based on the usual deterministic approach. Equation 1.11 is, for example, a complete analogy to the well-known rule for calculating the total resistance of series electrical circuits. The horizontal filtration along layers with fixed hydraulic heads at the ends of the interval of

interest in a confined aquifer is analogues to an electrical parallel circuit. So the hydraulic conductivity for evaluating the flux applying a homogeneous model must be the *arithmetic mean* of the hydraulic conductivity of the layers weighted with respect of their thicknesses.

There exist many ways for estimating errors of functions caused by errors of its parameters. Let a model represent by the function

$$y = f(x, P) \tag{1.14}$$

where x is an independent variable or a vector (list) of independent variables and $P = (P_1, P_2,\ldots, P_i,\ldots, P_n)$ is a vector (list) of the governing parameters. Then the errors of the model Δy caused by errors of the parameters ΔP can be estimated, for example, as

$$|\Delta y| \leq \sqrt{\sum_{i=1}^{n} \left(\frac{\partial f(x,P)}{\partial P_i} \Delta P_i \right)^2}$$

or

$$|\Delta y| \leq \sum_{i=1}^{n} \left| \frac{\partial f(x,P)}{\partial P_i} \Delta P_i \right| \tag{1.15}$$

Estimates 1.15 are provable only if Eq. 1.14 represents the phenomenon of interest adequately. If not all parameters affecting the modeled phenomenon are included in list P, then it can happen that Estimates 1.15 are acceptable still, if we are lucky, but the obtained errors are not provable.

If we had complete information on a geological object but for some reason were going to simulate its response on an impact, using simplified geological models, we could, at least in principal, evaluate the errors resulting from the simplification. However, if we simplify something that we do not know in full, we cannot evaluate the consequences of our simplifications. This is where, in my opinion, the central issue of hydrogeological modeling lies. Computer power at present is such that we are able to make predictions based on the highest theoretical level of the hydrogeological sciences (Beck 1987). However, there is a gap between the data necessary for making predictions and the available pertinent data. We do not know how accurate is the function $K(x)$ which we use in our simulations. Applying a piecewise homogeneous model, we can miss some homogeneous parts of the real site or add inexistent ones. We almost never know the exact locations of boundaries between the homogeneous parts and so on. We fill such informational gaps with assumptions. But "the modeling assumptions are generally false and known to be false" (Morton 1993; Beven 2005). Consequently, we cannot obtain provable estimates errors of the simulation result.

The use of false or not provable assumptions does not make the results necessarily wrong. They may be acceptable practically. For example, the Dupuit-Forchheimer simplification neglecting the vertical component of the Darcy velocity in all ours previous examples is wrong and contradictory. But as Muskat (1946)

observed that the resulting fluxes "will nevertheless be surprisingly close to those given empirically or by exact calculations". False or not tested assumptions do not permit provable estimations of the errors and uncertainty of the simulation results which are important for informed decision-making. However, they do not preclude achieving the best result and making the best decisions in some circumstances.

Two approaches to hydrogeological modeling exist at present. I call one of them engineering and the other geostatistical. The first approach is based on practical engineering experience. The second one is based on statistical methods which are developed to work with incomplete and erroneous data. The approaches do not exclude each other: the engineering approach includes some statistical features, and the geostatistical one uses the elements of the engineering approach essentially. Unfortunately, neither of them provides the provable estimates of the simulation result uncertainty as discussed in details in Chaps. 2 and 3.

"To do the best" (U.S. EPA 1987), we need first to define 'the best' reasonably, keeping our expectations in line with our possibilities. For example, we can request that our estimation must be the best one in the sense of the least squares method on a given monitoring network. Or it may be a subjective opinion of an expert based on his or her experience, what model and its parameters are the best in the given situation. After we defined meaning of 'the best', we need to furnish our model (models) with the set (sets) of values of the model parameters providing the best prediction in the defined sense. We are not able to evaluate the uncertainty of our best decision yet. But what we can do is to make our decisions more informed. It should not be one way to this end. Concept of one of them, based on transforming mechanisms and two-level modeling is suggested in this book (Chaps. 5–9).

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Chapter 2
Engineering Approach

In 1992, the journal *Advances in Water Resources* published a series of papers on validation of hydrogeological models. In one of those papers, Konikow and Bredehoeft (1992) hold that groundwater models cannot be validated but only invalidated. It means that the real quality of a model can be judged only by comparing the prediction that the model has produced with what have occurred actually, i.e., only based on post audit, and that the accurate results in process of model calibration do not warrant that the model will predict accurately. However, if calibration goes wrong, the model cannot be trusted. Commenting their paper, de Marsily et al. (1992) write:

> We all know that the parameters of a model are uncertain, probably wrong in many cases, and easily can be invalidated. Similarly, the 'structures' of the model (2-D, multi-layered, 3-D, etc.) can be incorrectly chosen. So what? As long as they reproduce the observed behavior of the system, we can use them to make predictions. It also seems to us that the better or the longer the reproduction of the observed behavior, the more confident we can be of their validity. … Using the model in a predictive mode and comparing it with new data is not a futile exercise; it makes a lot of sense to us. It does not prove that the model will be correct for all circumstances; it only increases our confidence in its value. We do not want certainty; we will be satisfied with engineering confidence.

Writing this chapter, I had a strong urge to call it "So what?" and to use as an epigraph the last sentence of the above quotation. But I overcame the urge and named it instead after the approach engineering. It is simple and transparent conceptually. Indeed, the modeling assumptions are generally "false and known to be false" (Morton 1993; Beven 2005). However working on many similar projects in similar geological surroundings and observing the results of implementation of those projects, professionals gain personal and collective experience of what models work satisfactory, how their parameter and boundary conditions should be assigned to yield the satisfactory results, and what is the chance that a given model fails which is a factual empiric estimate of the uncertainty of the simulation results. Validated in such probabilistic way, a model can be considered as "sound, fulfilling all necessary conditions, and just good enough model" (McCombie and McKinley 1993).

Let us come back to the models based on the Dupuit-Forchheimer assumption, that when the gradient of a water table is small enough, the vertical component of

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the Darcy velocity can be neglected and the flow considered as strictly horizontal. Such sort of simplifications is pretty common in mathematical physics or in engineering. Muskat (1946) calls the Dupuit-Forchheimer assumption "not trustworthy." However he expresses his astonishment by the fact that the results of its applications are accurate compared to "those given empirically or by exact calculations." Haitjema (1995) holds that "Dupuit-Forchheimer model could have done the job, saving resources and cost." Since the Dupuit-Forchheimer assumption is false, there is no possibility to evaluate the errors of the simulation results based on it in a closed way, i.e., based on errors of the model structure and its parameters. However Beven (1981) considers it reasonable for the water table slopes which are mild, and according to Bear (1972), it generates practically acceptable errors in homogeneous shallow aquifer on a horizontal aquitard, if the squared slope of the water table is less than 0.01.

Such use of not provable and even wrong assumptions, let us call them simplifications, which lead to accepted practically results under some empirically established conditions, I call the engineering approach. My attitude with respect to this approach is rather positive. It recognizes the reality, the impossibility to evaluate the uncertainty of predictions in a provable way. I would rather trust the professionals, though I understand that their experience is subjective and that it is different from an objective proof. However, this trust, though cautious, relates to the situations where the engineering approach really exists, e.g., in the case of building small reservoirs, or drilling water supply wells for small farms or family houses. However, what to do if there is no such experience, e.g., a project is unique per se, or unique for a given surroundings? Or what does one have to do, if experienced professionals make different recommendations and estimations?

Lerner (1985), described several cases related to the ground water supply in Africa, Latin America and England in which teams of highly qualified experts made different but equally incorrect estimations and predictions, using the same data. Anderson and Woessner (1992) report several instances with not so much encouraging results of post audit in the USA. They explain the failures by errors in conceptual models in developing which the professional experience plays the major role. Andersen and Lu (2003) add several more examples of post audits, that "have not provided high confidence in the predictive accuracy" of the applied models.

In relatively good times for the Soviet hydrogeology, an extensive study of the reliability of hydrogeological estimates of ground water resources was undertaken (Yazvin 1972). The study of 89 large intakes from artesian aquifers revealed that only in 12 cases the accuracy of the predictions was satisfactory. The resources were considerably underestimated in 76 cases and overestimated in one case. The study of 25 intakes from alluvial aquifers revealed that the resources were considerably overestimated in 20 cases. In all 114 cases the estimates of ground water resources were approved by the Central Commission on Ground Water Resources of the U.S.S.R. consisting of highly experienced hydrogeologists. In most of the above example, the professional expertise was combined with model calibration, and this fact aggravates the situation even more.

It may be consoling, at least in part, that the other fields where the completeness of geological information is essential share the same plight. One of the most well documented examples demonstrating that the uncertainty of geological modeling is not just an abstract issue is the complete failure of geophysical data interpretation relating to super-deep drilling at Kola Peninsula, Russia, (Kola 1984) and in Bavaria, Germany (Kerr 1993). As drilling revealed, actual geological structures differ completely from those anticipated. The same happened to the super-deep bore in Azerbaijan (Kola 1984). These failures cannot be explained by the scarcity of data or unsatisfactory qualifications of the interpretational teams. In such expensive enterprises as super-deep drilling, the teams certainly were the best, and the data (with respect to their amount and quality) exceeded what is available in routine enterprises. The failures were caused by the use of the "sound, fulfilling all necessary conditions, and just good enough" models recognized by the professional communities, but nevertheless fallible. Bredehoeft (2005) calls this "the conceptualization model problem" and gives several examples from his and his colleagues' hydrogeological practice in the United States. Problems, including civilian and economical, related to uncertainty of predictions made by experts in seismology are discussed by Geschwind (1997) and Hanks (1997), and many others. Unfortunately, professionalism and credentials do not always warrant the confidence in models and simulation results.

The view point that the engineering confidence is good enough to trust predictions is usually grounded on two groups of arguments. First, during their studies and professional activity, practitioners accumulate knowledge and develop thorough professional experience on where and how geological and mathematical models should be applied to yield practically meaningful results. We have discussed this kind of arguments above.

The second one is that all human progress is founded on the use of invalidated or even provably incorrect models. Indeed, it is true that "astronomers, on the basis of a few days of observations, will predict asteroid and comet orbits for thousands of years with good accuracy" (McCombie and McKinley 1993). Their argument can be even strengthen by mentioning one of the greatest achievement of those models: Le Verrier's discovery "on pen's point" of Neptune based on peculiarities of Uranus' orbit. He calculated the orbit of the unknown planet, and Neptune was discovered exactly at the location he predicted.

Somehow, it is less known that Le Verrier explained in the same way the peculiarities of Mercury's orbit (Levy 1973). This hypothesis was never confirmed. Its failure gave birth to several other hypotheses that failed also. It is recognized at present that Einstein's theory of relativity explains Mercury's behavior. My point is that there has never once been a need to revise astronomic models.

Effective modern technologies based on models which are impossible to validate can be included in this argument also. However, each such technology undergoes extensive testing, and then when it is applied, e.g., in manufacturing new products, special attention is paid to controlling the quality of raw materials, to assembly, and to other pertinent procedures. Final products are also tested. For example, each airplane and ship undergoes thorough tests before their practical use.

In hydrogeology we do not have such luxuries. Each hydrogeological site is unique. We cannot control its geological structure or even know the structure in full. Its response is also unique and depends on impacts. The impacts can be intensive and diverse, and many of them do not have analogs in the past. We do not have long enough periods of observations, and no prediction for a period of more than a 100 years has actually been tested. In science, if a hypothesis is proved to be wrong, another hypothesis takes its place, then another, and another, etc. In hydrogeology it may be too late to seek another model when it becomes clear that the applied one is faulty.

Professionalism is a necessary condition for obtaining meaningful results especially for development of geological models. As Tsang (1992) points out, a sick person should go to an expert having an M.D. degree. However, faith that the professional judgment is always true is also a fallacy.

Finally, let me repeat. If a professional has experience obtained on many similar projects in similar environmental and has observed the results of implementation of those projects, it could be reasonable to trust in the professional's judgment. Often such professionals do not need any mathematical modeling, they just know what works. (In Athens, Georgia, where I am typing these lines, I have never seen geological engineering or geotechnical explorations supporting projects for developing residential middle-class neighborhoods. The builders just know what kind of foundations must be used). However, in the case of the objects which are very expensive and carrying large environmental and financial risks, it is difficult if impossible to find a professional with the pertinent experience. Even if such professional exists, it is not reasonable to rely on his or her subjective opinion. We need models (quantitative theories) to predict what can happen, and of course we need professionals for developing conceptual geological models. However, if the professional's judgment about the uncertainty related to the use of some model in some situation is supported by the pertinent statistics, it should be taken in consideration. When such statistics is not available, nothing could be said about the quality and the uncertainty of the results obtained in the framework of the engineering approach.

However the contemporary computational technique and methods permit the development of a surrogate of the engineering experience. The surrogate cannot provide the provable estimate of the uncertainty either. But it permits more informed decision-making (see Chaps. 5–10).

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Chapter 3
Geostatistical Approach

The situation with the deterministic approach to predictive simulations is transparent. It can provide evaluations of the uncertainty of the simulation results in some typical circumstances for which the engineering experience does exist. Those evaluations are of the statistical nature. They are based on observed successes and failures of the decisions made based on results of the corresponding simulations. However, if such experience does not exist, the engineering approach fails to provide the provable estimates for the uncertainty of the simulation results. The situation seems more complicated with the geostatistical approach.

Statistics is the science which deals with incompletely known and fallible data which makes it so appealing to hydrogeologists (Shvidler 1963, 1964; Dagan 1986; Graham and McLaughlin 1989; Gomez-Hernandez and Gorelick 1989; NRC 1990; Review 1990; Cooley 2004; and many others). Thus, van Genuchten et al. (1990), write: "Because measurements and model predictions are both subject to uncertainty, the parameter estimation problem is essentially a statistical problem." More than this: geostatistics has come with the promise to quantify the uncertainty of the hydrogeological simulations: "…geostatistics has been integrated with hydrogeology to provide methods for quantifying uncertainty where estimation, interpolation, and extrapolation of hydrogeologic attributes are required between and beyond data locations" (Kitanidis 1997).

This widespread notion that statistics is a sufficient tool to overcome paucity of the geological data and provide provable estimates for uncertainty of the simulation results is a fallacy. Geostatistical estimates are strongly conditioned by many assumptions. As demonstrated below, some of those assumptions are impossible to test and some are known to be invalid. This means that the accuracy of the geostatistically acquired results cannot be proven. In this sense the deterministic and geostatistical approaches do not differ. Moreover, the geostatistical approach makes use of all or nearly all the assumptions of the deterministic one, plus many others. This alone makes it more vulnerable. Thus, averaging processes popular in geostatistical applications and resulting in the harmonic, geometric or arithmetic means of the actual hydraulic conductivity and transmissivity values are not related to the probability distributions of these properties. They emerge from deterministic formulations of some filtration problems as shown in Chap. 1. When a specific

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averaging process is defined (deterministically) and the probability distributions of the pertinent properties are known, then we can use statistical methods to estimate errors of those deterministically inferred parameters and the simulation results. So, if we reject the deterministic approach, the geostatistical estimates do not make sense. However, if we accept it, we can still doubt its geostatistical extensions, if they are based on unverified or knowingly false assumptions.

Even if statistical assumptions are valid, the geostatistical approach may be irrelevant. Thus, real ground-water flows always depend on the hydraulic conductivity and its variability. However, simulation hydraulic heads are not affected by the hydraulic conductivity, if the geological model is homogeneous, filtration is steady-state and governed by the Laplace equation with prescribed hydraulic heads as boundary conditions (Eq. 1.5). This shows that geostatistical formulations of some real problems can be meaningless. Therefore, before applying them, we must demonstrate their relevancy to the problem in hand. Mentioning the paucity and inaccuracy of the pertinent information is insufficient. It is the same situation as with numerical algorithms: not every algorithm is unstable, but because the unstable algorithms exist, we must demonstrate each time that the algorithm which we apply is stable when applied to the given problem.

It must be noted that the proponents of the geostatistics understand the artificial nature of introduction of geostatistics into hydrogeology. Thus, Review (1990) holds: "It should be noted here that the decision to select random functions to model a regionalized variable is only a matter of analytical convenience. This does not imply that the phenomenon under study is indeed random." Indeed, the hydraulic conductivity $K(x)$ in the problem leading to Eq. 1.1, reproduced here for convenience,

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

is unique for a given site and is not a random function. The fact that the measured values of $K(x)$ carry random errors does not make $K(x)$ a random function either. We can try to minimize the resulting errors in estimations of thickness $h(x)$ of the aquifer or of flux Q. To this end we could use a regression equation approximating $K(x)$ obtained by the least squares method applied to available observations on the hydraulic conductivity. In so doing, we are still in the frame of the deterministic approach. However, when we assume that $K(x)$ is a random function, we assume that what we observe within our site is only one realization of the function $K(x)$. Since we have only one, deterministic, distribution of the hydraulic conductivity the question arises: Where are the others? They must belong to other, analogous, sites. So we assume that our site is an element of an ensemble comprising many sites. The goal becomes to find stochastic characteristics of that ensemble and than apply them to our one. To solve this additional problem, we have to resort to a number of additional assumptions that can be as convenient and as false as the assumption that $K(x)$ is a random function.

Now let us assume that we have finally solved our problem. We got some result. It may be practically acceptable. Can we prove that our estimate of the uncertainty of our result is true? We can, if all our assumptions are true, but not, if even just one of them is false or untested. So let us consider some geostatistical assumptions and practice in more details.

3.1 Ensembles

The concept of an ensemble is basic for geostatistical approach (Dagan 1986). Conclusions, statements, and results of the statistical approach are related to ensembles or to their elements with respect to the ensembles. We estimate expected values of properties and the other statistics for an ensemble, the property's correlation and autocorrelation functions within the ensemble, the probability of a quantity characterizing an element to be within some range of the ensemble values of the same nature, etc. To evaluate an element belonging to an ensemble means to place it within the ensemble. To this end we must know statistical properties of the ensemble. If they are not known, but many other elements of the ensemble are available, we can try to use the available elements and statistical methods, to evaluate the ensemble properties and then proceed with the element of interest. However, in the geostatistical applications to hydrogeology, the site we have to work with is only one available element of an unknown ensemble. It is unique and it is not obvious where to look to find the others. To overcome this conceptual difficulty or, rather, to forget it, geostatisticians suggest that "the ensemble does not actually exist" (Dagan 1986).

The statistical approach does not make much sense if there is no ensemble. So we need to make up the ensemble, one element of which is our site. Since the unknown ensemble "is only a matter of analytical convenience", making it up is not an issue. Following to Dagan (1986) we assume that the made up ensemble is stationary (ergodic). This permits one to ascribe to the made up ensemble the statistical properties of the "random" functions observed at our site. Note that, even if an observed function exhibits some kind of stationarity within our site, the statement about stationarity of the made up ensemble is still just a hypothesis which is impossible to test, since only one element (one realization of the pertinent random functions) is available.

Thus, the site of the interest, the only available element of the made up ensemble, is assigned to be the mathematical expectation (the mean) of the made up ensemble. The flow within the site becomes the mean flow for the made up ensemble, and all geostatistical characteristics of the made up ensemble can be estimated based on the available observations on our site. In this way, we obtain, or rather make up, all necessary geostatistical data and can proceed with evaluating the uncertainty of the results of our predictive problem.

Unfortunately, for the reasons discussed in Sect. 3.5 and Chap. 4 and well known to geostatisticians, the use of the mean characteristics of an ensemble does

not warrant the mean response of the ensemble on a given impact. However, let us forget about this for awhile and ask the following question: How probably is that the only sample from an ensemble coincides with the ensemble's mean? The answer is obvious: not very. However, does this question make sense? For our convenience we constructed our made up ensemble in such a way that this should happen for sure.

However, what does one have to do, if a property, e.g., the hydraulic conductivity, as a function of coordinates, is not stationary obviously? No problem again: Dagan (1986) suggests generalizing the definition of stationarity "allowing for instance for polynomial trends and stationary increments".

The polynomial trend is the universal and most convenient tool for describing regional trends besides, maybe, the Fourier decomposition. We can try polynomials of different order until we find the polynomial that satisfies our taste. The only limitation is the maximal order of the polynomial, which depends on the number of available observations. The polynomial of the maximal possible order, though very attractive since its residuals equal to zero, is not stable with respect to additional data.

In general the mathematical description of a trend is a compromise between fulfilling the following requirements:

1. Reasonable considerations about a geological structure of the site.
2. Simplicity depending on amount of the available data and the intended application of the trend description.
3. Minimization of the sum of the squared residuals.

The first two of these requirements are obviously subjective. The third one follows from the first two. Thus, our judgment about the mathematical description of regional trends and even their existence are hypotheses that are impossible to prove. They may be more realistic than our hypotheses related to the random functions and the made up ensemble, but still remain hypotheses.

Figure 3.1 illustrates the possibility of polynomial trend descriptions (the data are from Bondarik 1974). Only polynomials of 1st, 2nd, 7th and 14th orders are presented in Fig. 3.1. The polynomial of the 14th order is not stable and the goodness of fitness criterion is not defined for it. Instead, we could use the linear interpolation between neighboring observations. However, then our regional trend becomes not differentiable at points of observation. Polynomial trends have the advantage of being differentiable everywhere.

So we can use fifteen polynomials, including the polynomial of the zero order, that is, the mean value of the observations, and many other mathematical representations to describe the regional trend and, according to Dagan (1986) convert our made up ensemble into stationary one. However, can we prove that our choice is correct? Even if some of the polynomials can be practically close within the region of interest, the situation remains the same: just the number of the alternatives decreases slightly. We would be also extremely lucky, if the true trend were presented in our set of the alternatives.

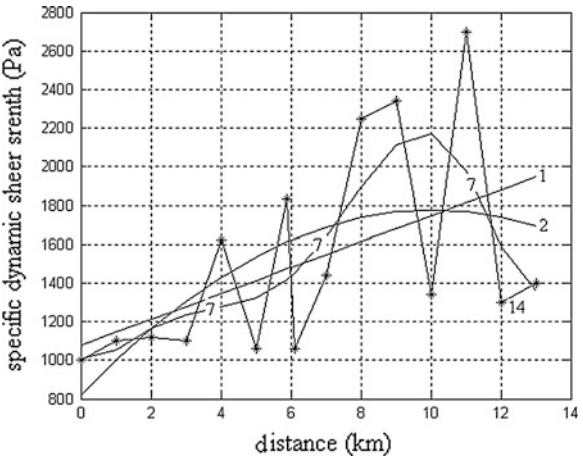

Fig. 3.1 Polynomial trends based on the factual data represented by *stars*

I do not know about you, but I feel some discomfort, since the made up ensemble remains arbitrary still. It seems that G. Dagan feels the same. So he recommends "to check a posteriori whether the stationary assumptions are met at a given degree of significance" and to use "some prior information derived from similar sites" (Dagan 1986).

I understand his first recommendation as testing the statistical homogeneity of the residuals. I doubt that we have enough data for real testing of statistical hypotheses in most cases and that such testing will make our choice less arbitrary. Indeed, there is nothing more statistically homogeneous than the residuals for the trend above presented by the polynomial of the 14th order with each residual equal to zero. However, do you believe that it represents the real trend? In general, the statistical testing of hypotheses is not a proof of their validity or invalidity. It only creates some basis for decision making which is arbitrary still. "A given degree of significance" means the probability to reject erroneously a tested hypothesis called usually the null hypothesis. However, the null hypothesis "is never proved or established, but possibly disapproved" (Fisher 1935). In other words, if a hypothesis passes statistical testing on a given degree of significance, it means, that we do not have enough evidence to reject it based on the criterion corresponding to the given degree of confidence. A number of different hypotheses able to pass the same test may exist. We know nothing about the probability of accepting the tested hypothesis when it is false. But namely this is essential for evaluating uncertainty of our simulation results (see Sect. 3.4).

Dagan's suggestion to use "some prior information derived from similar sites" seems to be an attempt to include the only available element in a really existing ensemble and is a good idea. To do this, we must define what similarity of hydrogeological sites and impacts means, how it can be evaluated, and already know similar sites and their responses to the impact at hand. To my knowledge the method of geological analogy (Rozovsky and Zelenin 1975) is the only example of such approach. Interesting conceptually, it has few practical applications, since it

requires the existence of similar sites with similar impacts and already observed responses to those impacts.

Thus, we are able to make up a number of ensembles to which our site could belong. However, this does not change the situation: the choice of the ensemble remains an untested hypothesis.

3.2 Elements

Ensembles are collections of elements. The elements are bearers of properties or characteristics. Thus, when statisticians study the height, weight or longevity of a population, the elements are human beings. When they study income, the elements can be families, and so on. To make the results more accurate and interpretable, statisticians make the ensembles as statistically homogeneous as possible: they partition the ensembles by gender, race, age, the number of the families members, level of income, etc. The fictitious analogues site discussed in the previous section are also elements characterized by different random functions. Since geostatisticians consider all such elements to be analogous to the site at hand, let us restrict ourselves with properties within the site only.

In geology and, in particular, in hydrogeology the role of the element carrying a property is assigned to the representative elementary volume (REV). Following the established tradition (Kolomensky and Komarov 1964; Bear 1972; Brown et al. 2000), let us introduce the notion of REV using porosity. In principle, porosity can be measured on slices of media, applying the Bernoulli trail. That is, if a point selected at random falls into a pore, the result of the measurement x_i is assigned equal 1 ($x_i = 1$), otherwise $x_i = 0$. If we repeat this procedure n times, than the porosity θ of the sample is evaluated as the mean of the measurements: $\theta = \frac{\sum_{i=1}^{n} x_i}{n}$. Its variance, $\sigma^2 = \frac{\theta(1-\theta)}{n-1}$, decreases with increasing of the number of the measurements. The standard procedure of evaluating porosity on samples of a finite volume is more convenient, since each such evaluation substitutes for manifold of the measurements on the slices. Nevertheless, the variation of the porosity depends on the sample's volume still. A possible pattern of changing of the mean porosity estimates yielded by the samples of different volumes is shown in Fig. 3.2. The volume of the samples for which the variance of the porosity becomes negligible is assigned as REV. If we continue to increase the sample volume, the mean or the mathematical expectation of porosity can start changing again. These changes are usually attributed to the fact that the volume becomes too large and includes some heterogeneous macroscopically changes in the structure of the media. It becomes statistically and geologically heterogeneous.

The notion of REV defines the element bearing a property, its point value, and makes the property as if continues in space. It is possible that different representative elementary volumes exist for different properties. In such case the issue can emerge whether to assign the same REV for all pertinent properties and how to

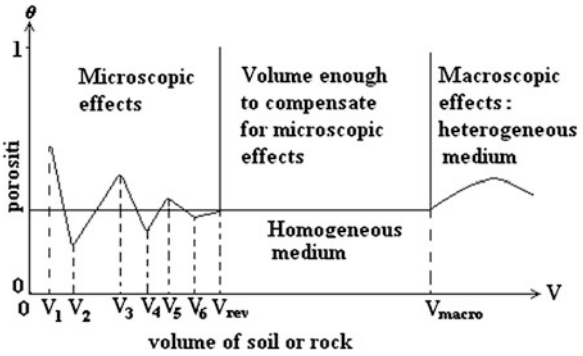

Fig. 3.2 Definition of representative elementary volume for porosity

make the choice or to use different REV for different properties which could be inconvenient.

In the case of porosity, changing the sample volume leads to changing of the variance σ^2. This phenomenon is called by Rats (1968) "*scaling effect of the second kind*." It is well known to statisticians (Yule and Kendall 1950). Some properties have "*scaling effect of the first kind*" (Rats 1968). The means of such properties depend on the volume of samples on which they are measured. For example, the mean of the strength of soil and rocks decreases with growth of the sample volume (Kolomensky and Komarov 1964) and the mean of the hydraulic conductivity increases with growth of the sample volume (Rats 1968). According to Bolotin (1969) the strength of a sample is defined by the weakest element of its structure. The probability to have such elements in a sample increases with sample size. Rats (1968) extended this explanation to the hydraulic conductivity: the hydraulic conductivity is defined by the most conductive element in a sample. The probability to find such structures within a sample is larger for larger samples. One of the Weibull probabilistic distributions relates the mean of the hydraulic conductivity obtained on samples of volume V with the mean conductivity of a reference sample of volume V_0. Thus, the results obtained by testing different volumes of soils and rocks may be different statistically even for statistically homogeneous media just because of differences in the volumes of samples. This can cause some problems with defining the REV.

The notion of REV is convenient in laboratory studies when the volume of samples can be controlled. But here we are most interested with the cases when we can control neither the volumes nor the shapes of bearers of the obtained results, as happens, for example, in pumping tests. To deal with such situations Rats (1968), Dagan (1986), and many other hydrogeologists suggest a simple and straightforward approach. They introduce different scales of heterogeneity and use these scales as elements of corresponding ensembles. Thus, Dagan (1986), speaking about the hydraulic conductivity, writes that a point in the *local scale* has dimension of the order 10^{-1}–10^{0} m. These points are characterized by results obtained on extracted cores and by slug tests. In the *regional scale*, according to him, a point has dimension of the order 10^{1}–10^{2} m.

Such assigning of the elements carrying a property values is arbitrary in essence. Thus, it is not clear why the results yielded on cores are of local and not of laboratory scale. Pumping tests involve different volumes of soils and rocks, depending on geological settings, duration and patterns of the tests and interpretation models. For example, three-hour, three-day, three-week, and three-month pumping tests involve different volumes of geological media. Then the question arises: should or should not we introduce different scales for the results of the pumping tests of different durations, and if we should, how many scales should we have and how we define them? The results of pumping tests depend on interpretation models. We can arbitrary change those and have different results and bearers of the hydraulic conductivity or transmissivity. Say, if we consider an aquifer as a homogeneous, unconfined in plane, and assign the boundary conditions in infinity, then the resulting hydraulic conductivity or transmissivity formally relates to the entire aquifer which is not realistic. If we had a developed monitoring network, we could limit the infinity by the distances to the furthest monitoring wells that do not respond to the pumping. Without such network, we can do what usually geophysicists do, namely to call infinity the distances exceeding the thickness of the aquifer in ten times, or something similar. If we apply a different interpretation model, say a pumping test is conducted near a river well connected to the aquifer, we may have quite different situation. When the hydraulic conductivity and transmissivity are defined by model calibration, the elements bearing the results of calibration depend on structures of the calibrated models and the model identification problem formulation (Gorokhovski 1977; Yeh and Yoon 1981; Yeh 1986).

The scales and their interaction are confusing, at least, for me. So, it is interesting to see how geostatisticians deal with them. For example, Zimmerman et al. (1998) use in their work estimates of the hydraulic transmissivity at 41 boreholes obtained through slug tests, local pumping tests, and three regional-scale pumping tests lasted from 1 to 3 months. The obtained transmissivity values span 7 orders of magnitude, from 10^{-7} to 10^{0} m^2/s. Nevertheless all these transmissivity values are considered as a collection coming from the same ensemble (Zimmerman et al. 1998, Table 2a). Thus, the scaling is just ignored. I assume that this was done because it was impossible to infer serious statistical conclusions from the results obtained through three regional-scale pumping test. The same happens if we separate slug tests and local pumping tests. (I do not believe that serious statistical conclusions can be supported by 41 available values either.)

By the way, Zimmerman et al. (1998) state: “Large-scale pumping tests indeed suggest that narrow, relatively conductive fractured zones are possible in some areas.” This is possible. However, it seems a strange coincidence that all three large scale pumping tests occurred within “narrow, relatively conductive fractured zones.” It could be suggested as well that the larger transmissivity values are due to the scaling effect of the second kind. It would be interesting to compare those three conductivities with the conductivities obtained for the same zones by slug tests or laboratory measurements. Anyway, both above explanations contradict to the statements of Dagan (1986), Moore and Doherty (2006), and many others that the results of the regional pumping tests are statistical averaging of locally scaled

properties, that is, the regional-scale conductivities are not weighted averages of the smaller-scale ones with not negative weights summing to one. Review (1990) recognizes the existence of negative weights: "Negative weights (often, but not always) occur for points that are "shadowed" by closer points." The authors do not explain what exactly "shadowed" means and why the negative weights occur. Isaaks and Srivastava (1989) relate the appearance of the negative weights in their Eq. 17.1 to the values of secondary data without any explanation what the "secondary data" means. The appearance of the negative weighting factors follows from Eq. 8.25 presented by Kitanidis (1997) also without explanation. (The mechanism of the appearance of the negative weights is demonstrated in Chap. 5.)

Unfortunately, the notion of an element in hydrogeological geostatistics is as vague as the notion of an ensemble. Both are "a matter of analytical convenience".

3.3 Sampling at Random

Sampling at random is one of the most important requirements for making provable statistically inferences. But what is sampling at random? Gnedenko (1963) writes that "many authors have arrived at the conviction that in the case of infinite number of outcomes, no definition of probability can be given that is objective and independent of the method of calculation." He gives several examples of the problems which, depending on the operational definition of sampling at random, lead actually to different problems with different solutions and describes the real-life situations relevant to each solution. One of them, called the Bertrand's paradox, is cited here.

The problem is formulated as following: A chord of a circle is chosen at random. What is the probability that its length exceeds the length of a side of the inscribed equilateral triangle?

Case 1 By consideration of symmetry, the direction of the chord can be fixed at point A in advance. The chords of this direction exceed the length of a side of the inscribed triangle if they intersect the diameter that is perpendicular to them within interval CC′ (Fig. 3.3, Case 1). The length of this interval is equal to radius of the

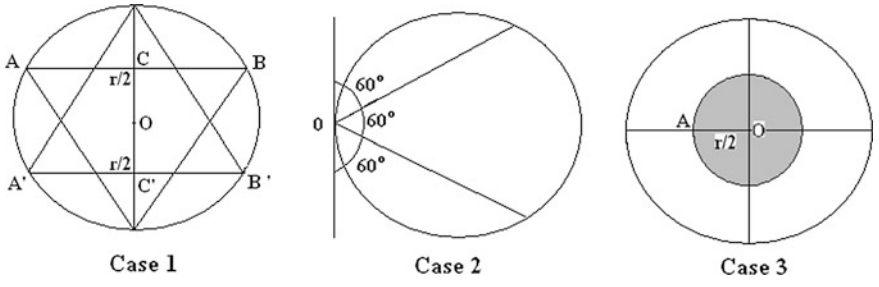

Fig. 3.3 Bertrand's paradox

circle, r. Since the diameter of the circle is $2r$, the probability for the chord length to exceed the side of the equilateral triangle is equal to 1/2.

Case 2 As in Case 1, we can fix one end of a chord in advance. The tangent to the circle at this point and two sides of the inscribed equilateral triangle with vertex at this point form three angles, each equal 60^{o} (Fig. 3.3, Case 2). Only the chords falling within the middle angle are favorable cases. Thus, by this method of computation, the probability we are looking for is equal to 1/3.

Case 3 We also can fix the positions of a chord by indicating its midpoint position. For chords to exceed the length of a side of the inscribed equilateral triangle, their midpoints must lie within the concentric circle with radius $OA = r/2$ (Fig. 3.3, Case 3). The aria of this circle is equal to 1/4 of our circle. Therefore, the probability we are looking for is equal to 1/4.

Depending on how the notion "at random" is defined, we actually have three different problems with three different solutions. Gnedenko (1963) provides the real life situations relevant to each of these three formulations of the notion "at random".

Thus, good practice would dictate that when formulating a geostatistical problem, the sampling at random must be defined operationally, and its relevance to the problem formulation must be demonstrated. This is never being done in hydrogeology. Moreover, the sampling systems in hydrogeology are almost never random. They are based on the professional experience and understanding of hydrogeological surroundings. Thus, prospecting ground water resources, hydrogeologists allocate wells where they anticipate finding water. They do not conduct pumping tests where low hydraulic conductivity is suspected. This is a sound and effective hydrogeological practice. But the results based on such sampling systems are not representative statistically: they are biased.

3.4 Probability Distributions

About all theoretical and practical developments of geostatistics in hydrogeology are based on the assertion that the hydraulic conductivity and transmissivity have the lognormal probabilistic distribution. The assertion is very convenient, greatly simplifying calculations. However, it reminds the well known joke that physicists consider that the universality of the normal distribution of probability is a theorem proven by mathematicians, while mathematicians think that it is an empirical law established by physicists. Likely, hydrogeologists and geostatisticians relate to the lognormality of the hydraulic conductivity in the same way.

In fact, according to Review (1990), there exist many different probability distributions of the hydraulic conductivity and transmissivity. Thorough studies conducted in the Soviet Union (Borevsky et al. 1973) have revealed that probability distributions of the hydraulic conductivity can be divided into three

approximately equal groups: normal, lognormal, and those which could not be described as normal or lognormal.

As discussed above, the volumes characterized by the values of the hydraulic conductivity are known only if they obtained in the laboratory tests. The elements characterized by the hydraulic conductivity values obtained by slug and pumping tests are not. Their volumes and shape depend on duration of the tests and the geological surroundings Then the hydraulic conductivity of what do the probability distributions describe?

The common assertion that the hydraulic transmissivity has the same distributions as the hydraulic conductivity just adds confusion. For example, in the case described by Zimmerman et al. (1998) both have the lognormal distribution of probabilities. However, the transmissivity is a product of the conductivity and the thickness of the aquifer. Therefore, the thickness should have some special distributions for the product of the thickness and the conductivity to have the same kind of the probability distribution as the conductivity. I never heard about a study of the probabilistic distributions of the thickness of an aquifer or aquifers.

Statements about distributions of the hydraulic conductivity are based usually on testing the hypothesis about its probabilistic distributions at "a given degree of significance". Let us consider this procedure more closely. Let an ensemble consist of the elements bearing random values of property X. We assume that the probability density function of X is $p_0(x)$ (Fig. 3.4). To test our hypothesis, call it H_0, we perform the following simple procedure. We assign some criterion x_α. Then we sample the ensemble at random. The obtained sample is characterized by value x_s. If $x_s > x_\alpha$, we conclude that our hypothesis that X has the probability density function $p_0(x)$ is wrong and reject it. Otherwise we accept the hypothesis.

In practice we usually assign not x_α, but α, the degree of significance,

$$\alpha = \int_{x_\alpha}^{\infty} p_0(x)dx \tag{3.1}$$

and calculate x_α, based on Eq. 3.1. In technical applications the degree of significance is usually assigned as 0.1, 0.05, or 0.01. If our selection of the sample has been random, than the probability to obtain $x_s \geq x_\alpha$ is small. We expect that an

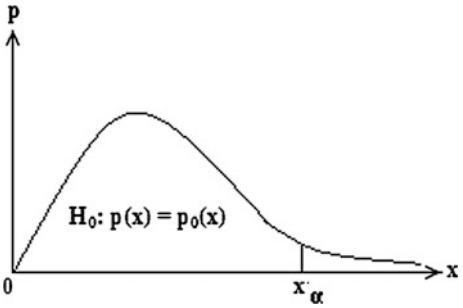

Fig. 3.4 Testing hypothesis H_0 based on a degree of confidence

event with low probability is not likely to happen in a single experiment. But it has happened. Therefore, our assertion that value x_s has a low probability likely is wrong. So we reject the hypothesis that X has the probability density function $p_0(x)$.

However, rare events happen from time to time, and rejecting hypothesis H_0, may be a mistake. The probability of such mistake is α. The degree of significance is the probability to reject erroneously the hypothesis which we are testing when it is true. In doing so, we commit so called a *type I error*. Obviously, assigning the degree of significance is arbitrary. If we are critical with respect to the hypothesis, we can increase α, moving our criterion x_α to the left. It makes rejecting the hypothesis more probable. If we like the hypothesis, we can decrease α and move x_α to the right. This decreases the probability of making type I error. Anyway, assigning some degree of significance, we establish the criterion for recognizing whether the obtained evidence is sufficient to reject our hypothesis and not more than this.

However, what does a degree of significance say about the possibility of committing a *type II error*, i.e., accepting hypothesis H_0 when it is wrong? The answer is not much. Common sense suggests that in our case, by moving x_α to the right and decreasing α, we relax the condition to accept our hypothesis. Therefore the probability, β, of type II error is increasing. If we increase α, moving x_α to the left, we increase the probability of type I error, and decrease the probability of type II error. That is all. We cannot evaluate β in a quantitative way unless we have the probability density function $p_1(x)$ of an alternative hypothesis H_1.

Let us assume that we have alternative hypothesis H_1 with the probability distribution function $p(x) = p_1(x)$ (Fig. 3.5). Only one of these two hypotheses is true. The procedure of testing the hypotheses is the same as above. We assign a criterion. It seems to be natural, but not mandatory, to pick as the criterion value x_{01} for which $p_0(x_{01}) = p_1(x_{01})$. Then we sample at random ensemble and obtain the sample for which $x = x_s$. If $x_s > x_{01,}$ we conclude that hypothesis H_0 is wrong, reject it and consequently accept hypothesis H_1. If $x_s < x_{01,}$ we accept hypothesis H_0, rejecting hypothesis H_1. The probability of erroneously rejecting hypothesis H_0, the probability of type I error, is

$$\alpha = \int_{x_{01}}^{\infty} p_0(x)dx \tag{3.2}$$

The probability to reject erroneously hypothesis H_1 is equal

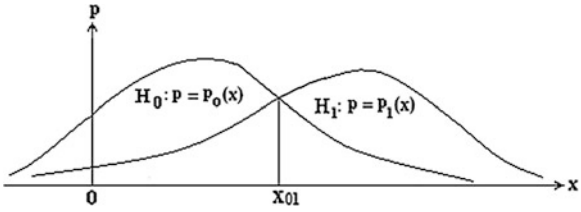

Fig. 3.5 Testing hypothesis: simple alternative

$$\beta = \int_{-\infty}^{x_{01}} p_1(x)dx \tag{3.3}$$

Erroneously rejecting hypothesis H_1, we erroneously accept hypothesis H_0. Therefore β is the probability of type II error, to accept erroneously hypothesis H_0 when it is wrong. So the probability for hypothesis H_0 to be true is equal to $1 - \beta$. This value is called the power of the criterion.

Our choice of value x_{01} does not consider the further use of the obtained result. Having some additional information, we can select a different value x_{01}. If we move x_{01} to the right we decrease the probability of type I error, but increase the probability of type II error. If we move it to the left, we get an opposite effect: we increase the probability of type I error and decrease the probability of type II error. If we knew the losses ($loss_\alpha$ and $loss_\beta$) associated with errors of both types, we could formulate the problem of finding x_{01} as a problem of optimization. That is, we could select x_{01} in the way minimizing the goal function, representing the mathematical expectation of the losses:

$$loss = \alpha\, loss_\alpha + \beta\, loss_\beta \tag{3.4}$$

This provides about the most objectivity we can achieve, performing hypothesis testing in the case of a simple alternative.

The hypothesis testing becomes more complicated in the case of many possible alternatives. It would be solvable still, if we could compile a complete list of alternatives weighted by their probabilities to be true. Say, we assume that the hydraulic conductivity has a lognormal distribution. But what is the complete list of the mutually incompatible alternative to our hypothesis? And how can we weight the hypothesis, including H_0, to be true?

The point here is that making a choice based on a given degree of significance, we cannot evaluate uncertainty associated with the choice. We do not know to what elements values of the hydraulic conductivity relate, cannot compile the complete list of the possible alternatives of the probability density functions and formulate objectively the objective function for making the choice. Therefore, we never know the probability that the accepted hypothesis is false. Or coming back to the contest of evaluating uncertainty of the results of hydrogeological modeling, we never know the uncertainty associated with the acceptance of our hypotheses. This relates to all parameters involved in the underground water flow.

3.5 Effective Parameters

To produce predictions related to underground flow and contaminant transport based on solving pertinent mathematical equations and their systems (mathematical models), we have to know coefficients of the mathematical models continuously,

that is, at each point of the geological object of interest and at each instant of the period of the predictions, as well as the corresponding initial and the boundary conditions. Since it is impossible, the simulation results never reproduce reality exactly. In the geostatistics approach the goal is reproducing an average behavior of all processes of interest related to the underground flow: the hydraulic heads, fluxes, contaminant plume contours, travel times, etc. It is assumed that this can be achieved, using some lump values of the pertinent parameters. Thus, instead of non-countable (infinity large) sets of property values, their small finite amount could be used (Cooley 2004). These values are called effective parameters. Since the goal of the geostatistical approach is to predict some average behavior of the underground flow, it seems to be natural to use some statistics of the pertinent characteristics as effective parameters.

It was believed on the early stage of the geostatistics development, that the statistically inferred effective hydraulic conductivity is effective in a broad spectrum of hydrogeological situations, since "if there is no unique best effective hydraulic conductivity…, the predictive capability of the model must be questioned" (Gomez-Hernandez and Gorelick 1989). Dagan (1986), defining the effective conductivity as the value that satisfies exactly the Darcy law for uniform steady-state average flow, holds that the effective hydraulic conductivity, K_{ef}, is bounded with the harmonic mean, $K_H = exp\left(\mu_Y - \sigma_Y^2/2\right)$, and the arithmetic mean, $K_A = exp\left(\mu_Y + \sigma_Y^2/2\right)$, where μ_Y and σ_Y^2 are the geometric mean and the variation of the natural logarithms of the observed values of the hydraulic conductivity K:

$$K_H \leq K_{eff} \leq K_A \tag{3.5}$$

He also holds that for three-dimensional flow in isotropic media

$$K_{eff} = K_G\left(1 + \sigma_Y^2/6\right) \tag{3.6}$$

($K_G = exp\,(\mu_Y)$ is the geometric mean.)

Dagan (1986) states that Eq. 3.6 "is of a rather academic interest," since "we generally measure directly a space average of K by pumping tests" and "under certain limiting conditions, yet to be elucidated in a quantitative manner, this space averaging is close to K_{ef}." Equation 3.6 and the above Dagan's statement seem strange for me. A regional pumping test averages properties on local scale (the elements with size 10^{-1} to 10^{0} m) in radius 10^{1} to 10^{2} m. Let an impermeable boulder or even a pebble be among the local scale elements being averaged. The result of such averaging is $K_G = 0$. Thus, just a pebble makes a regional hydraulic conductivity equal zero. May be for this reason Dagan (1986) writes about "certain limiting conditions" which are not elucidated yet.

Nevertheless, the concept that the results obtained by pumping tests on some scaling level are averages of the hydraulic conductivity values, belonging to the

preceding scale level is shared by most of geostatisticians (Review 1990; McLaughlin and Townley 1996; Cooley 2004; Moore and Doherty 2006, and many others). However, as mentioned above, the results of pumping tests depend on the chosen interpretation models, which are arbitrary in principle. It is hard to believe that the choice of the interpretation model does not affect the character of "the space averaging."

The anxiety of Gomez-Hernandez and Gorelick (1989) that a unique value of the effective hydraulic conductivity may not exists, happened to be justified. Beven (1989) writes that many studies "have concluded that it is not possible to define a consistent effective parameter value to reproduce the response of a spatially variable pattern of parameter values." Neuman and Orr (1993) showed that "an effective hydraulic conductivity does not generally exist." They also "demonstrated numerically that in two dimensional mean radial flow an effective hydraulic conductivity may increase from the harmonic mean of $K(x)$ near interior and boundary sources to the geometric mean far from such sources." But contrary to the statement of Gomez-Hernandez and Gorelick (1989), the predictive capability of predictive models is not questioned by geostatisticians.

Cooley (2004) recognizing the absence of unique effective values of the hydraulic conductivity, explains it, as do many other geostatisticians, with the fact that hydrological mathematical models are nonlinear with respect to the hydraulic conductivity. To understand this, let us consider a simple example. Let some variable of interest q be a linear function of the property k:

$$q = ak + b$$

Let k take values k_1 and k_2. Then the arithmetic mean of q is

$$\overline{q} = \frac{ak_1 + ak_2 + 2b}{2} = \frac{ak_1 + ak_2}{2} + b = a\frac{k_1 + k_2}{2} + b = a\overline{k} + b$$

So we can evaluate the arithmetic mean value of $\overline{q}$ and its statistical characteristics applying the arithmetic mean value $\overline{k}$ and its statistical characteristics. Thus, $\overline{k}$ and $\overline{q}$ are effective statistically and $\overline{k}$ provides the effective value $\overline{q}$.

Now let variable h be a quadratic function of k:

$$h = ak^2 + b$$

Then the arithmetic mean value $\overline{h}$, is not equal to its estimate $\hat{h}$ calculated with the use of the arithmetic mean $\overline{k}$:

$$\overline{h} = \frac{ak_1^2 + ak_2^2 + 2b}{2} = \frac{a}{2}\left(k_1^2 + k_2^2\right) + b \neq a\overline{k}^2 + b = a\left(\frac{k_1 + k_2}{2}\right)^2 + b = \hat{h}$$

Indeed,

$$\overline{h} - \hat{h} = \frac{a}{2}\left(k_1^2 + k_2^2\right) - a\left(\frac{k_1 + k_2}{2}\right)^2 = \frac{a}{4}\left(k_1^2 - 2k_1k_2 + k_2^2\right) = \frac{a}{4}(k_1 - k_2)^2$$

Unless $k_1 = k_2$ or $a = 0$, making h constant, $\overline{h} \neq \hat{h}$, due to non-linearity of mathematical models. Thus, though $\overline{k}$ is the effective statistics for k_1 and k_2, it is not effective parameter for evaluating h. So, different variables of interest can require different effective values of the same parameters. Of course, this example is oversimplification of the real life situations, just to demonstrate in the simplest way how non-linearity works.

No doubt, the nonlinearity hydrogeological processes contributes to the fact that the effective parameters are not universal. However, this obstacle can be overcome, for example, by the use of the Monte Carlo method (Shvidler 1963, 1964). The real issue is still the paucity of data on structures and properties of geological objects. We cannot know how what is unknown can affect the effectiveness of the parameters which we for some reason assigned as effective. Even different formulations of simulation problem on the same object can require different effective parameters (Gorokhovski 1977, 1996; Yeh and Yoon 1981; Yeh 1986; Beven 1989). This phenomenon is called *problem dependence of model identification*, since it was revealed in process of calibration of predictive models. Therefore, if even the effective hydraulic conductivities of hydrogeological models were statistics, which in general is not true (see Chaps. 5–7), they should be different statistics for different formulations of simulation problems.

3.6 Meaning of Geostatistically Inferred Results

Let us assume that all our geostatistical assertions about the site of interest are true and that we have obtained true results. What do they mean really? For example, an insurance company evaluates the average longevity for a segment of population and does this correctly. However, can the company predict what will happen to a person with the average characteristics of a given segment of the population? The answer is no. The segment of population to which my parents and my talented colleague belonged had the average longevity about 60 years. My parents passed away at age 89 and 92 years and my colleague at 40 years.

Meteorology, with its much longer historical records, numerous comparisons of statistical generalizations with real facts, and much better developed observational networks and predictive techniques than hydrogeology, makes a quite expressive illustration of this point. Thus, a 100-year flood event statistics refers to the disastrous floods which in a long sequence of years occur in average once per a hundred year, that is, it has the probability equal to 0.01 to happen during a one-year period. Nevertheless two such floods have happened in California just during first three months of 1995 and then again in 1997. The possibility that the climate change or some other factors depriving the long previous series of observations of the statistical meaning for the future predictions makes the situation even worse.

In the same way, the geostatistical approach, if all its assumptions are true, leads to the results that represent the average response of the made-up imaginary

ensemble. They do not relate to the unique object used to make the ensemble up, and to what can happen to the object.

3.7 Geostatistics and Uncertainty

As Hornung (1990) puts it, "One cannot substitute lack of theory and/or data by sophisticated mathematical models for parameter identification." Developing such complex theories, as hydrogeological geostatistics or proving new and beautiful theorems are challenging, and gratifying. However, how practical are those achievements? V. N. Tatubalin, a colleague of A. N. Kolmogorov and B. V. Gnedenko in the Department of the Probability Theory, Moscow State University, U.S.S.R., who often consulted hydrogeologists and geological engineers in 1960s and 1970s used to say: "You are looking for a razor. But considering amount and quality of your data, you would better learn to work with a chopper."

Shvidler (1963, 1964), one of the pioneers in application of random functions to underground flows, gives the best, to my knowledge, practical example, applying them to oilfields consisting of 60–80 wells located on a relatively small territory. He describes the procedure of geostatistical solving the filtration problem in the following way (his notation is substituted with the one used in this text):

1. From experimental data one realization of random function $K(x)$ is constructed.
2. From one realization, the appropriate functional characteristics—mathematical expectation and autocorrelation functions of (the hydraulic conductivity) $K(x)$—are determined.
3. Based on them sufficiently many realization of $K(x)$ are constructed.
4. Any algorithm whatever for solving the corresponding boundary value problem for each realization of $K(x)$ is applied.
5. From the set of boundary values solutions obtained the fundamental characteristics of the random function $h(x)$ are computed.

To realize steps 1–3, he applied the assumptions of stationarity of the observed random function $K(x)$ suggested later by Dagan (1986). To realize step 4, he applies different algorithms including analytical or numerical solutions, the method small perturbations, the random walk, and the Monte Carlo simulations, all of them in the deterministic mode. Step 4 provided also the solution of the problem of nonlinearity of the original deterministic problem. In Step 5, Shvidler usually restricted himself with calculating the mean and the variations of the yield of the oil pumping wells. The latter was usually based on the Chebyshev inequality: if $\lambda > 1$ is an arbitrary positive real number, q is a random variable, $\overline{q}$ is its mean, and σ_q is its standard deviation, than the probability of the event $|q - \overline{q}| > \lambda\sigma_q$ is smaller than λ^{-2}, that is,

$$P\{|q-\overline{q}|>\lambda\sigma_q\}<\lambda^{-2} \tag{3.7}$$

The Chebyshev inequality does not depend on the probabilistic distribution of the random variable q and permits evaluating two-side confidential intervals for a given confidence level and vise versa, though it overstates the confidence levels. For example, an arbitrary distributed variable q lies in the interval $\overline{q}\pm 3\sigma_q$ with the probability close to 0.9.

Shvidler states also that it is necessary to have tens and in some cases even hundreds of observations for reliable derivation of correlation functions. (In his real-life examples, the number of observation wells is always above 60.) Since in many cases, we do not have sufficient information for a valid determination of the statistical characteristics of the random functions, we have to choose between the deterministic and stochastic approaches. However, he writes: "It is quite obvious that the statistical model should be preferred as being more general." It may be, but not for me.

Shvidler (1963, 1964) never mentioned that the statistical approach provides provable estimates of the uncertainty of its results. He rather considers it as a way to systematize and optimize modeling: Steps 1–3 above are preparations to step 4 which is deterministic essentially. It is possible that the geostatistical approach can be useful in this sense sometimes, for example, in a context of model equifinality (Beven and Freer 2001). However, what is discussed here is not the comparison of the computational efficiency of the two approaches but the inability to obtain the provable estimates of uncertainty of the results of the engineering approach and, as if, the ability of the geostatistical one to provide such estimates.

It is a common and sound practice in mathematics to use convenient assumptions and methods such as the Lagrange multipliers or the perturbation methods to facilitate analytical solving of many problems. When analytical solutions are impossible, finite difference and finite element methods are convenient tools to yield numerical solutions. Statistical concepts and Monte Carlo simulations are used sometimes as a tool to solve deterministic problems such as evaluating integrals and solving differential equations. The Buffon needle problem of the value of π estimation is a famous example of the Monte Carlo method application (Gnedenko 1963; Gentle 1985). However, all such applications include demonstrations that the employed conveniences actually lead to the solutions of the original problems, that is, the yielded solutions converge to the true solutions if the number of experiments or nods, in case of numerical methods, goes to infinity.

This is not the case for hydrogeological applications of geostatistics in which the word random is like the magic spell "open sesame": one proclaims whatever one wants as random and then is free to proceed. In geostatistics the analytical convenience means a complete substitution of the problem needing solution by a vaguely related problem which seems easier to solve. The deterministic problem of finding space–time distributions of the hydraulic heads caused by a given impact within a given site is replaced by the problem of evaluating the average

distributions of the hydraulic heads or fluxes belonging to a made-up ensemble. The reason for the substitution is the impossibility of estimating the error of the results from the deterministic formulation of the problem. To solve this new problem, an ensemble is made up which consists of undefined elements and actually even does not exist, random functions are applied to the phenomena which are not random, and many assumptions are employed which are not properly tested, or not tested at all, and "generally false and known to be false" (Morton 1993; Beven 2005).

The geostatistical approach may render the results accepted practically. However, contrary to statements of geostatisticians, it does not permit evaluating the uncertainty of those results in a provable way. Thus, one of their most power tools to overcome non-linearity of hydrogeological models and complications with defining statistical distributions of the simulation results is the Monte Carlo simulations. Let us forget that expressing the simulation result uncertainty in terms of levels of significance without evaluating type II error is meaningless. The main problem with such use of the Monte Carlo simulations is that their object is a model itself but not its relation to the real world (Gentle 1985). Varying the parameters of a model, one can evaluate the model sensitivity to its parameters, but and not more than this.

I do not think that all this is news for geostatisticians, at least for those from the first generations. I cited above works of Dagan (1986) and Review (1990) where they stated directly that they introduce most of their assumptions not because they are true, but because they are convenient. However, Kitanidis (1997) motivates the next generation of geostatisticians, claiming that "because we cannot come up with a deterministic mechanism that explains variability, we postulate a probabilistic model", that the common sense "is often the best guide" and that geostatistics are "practical and reasonable way to use what we know in order to make predictions". He recognizes that the geostatistical technique may be misleading and should be avoided if certain assumptions are not met. Based on the common sense, he suggests considering an assumption as met if it is reasonable, there are no evidences to contrary, and the data do not discredit the assumption.

All of these and even more have been already discussed above. However, the two following suggestions seem to be new. First, Kitanidis (1997) suggests, based on the common sense and the geostatistical traditions, to use, the Fourier decomposition "to grasp the concept of scale" for the properties varying in space. The Fourier decomposition representing a function as a sum of infinite number of harmonics of different periods and amplitudes is a powerful and widely used tool in both pure and applied mathematics. But if we take in consideration that about any trend, including linear and polynomial, can be subjected to the Fourier decomposition, it becomes obviously that the Fourier decomposition has nothing to do with the concept of scales. Applying such logic, we can use the Taylor expansion to grasp the linear, quadratic, cubic and so on components (or scales?) of the regional trend. Mathematics permits describing trends as sums of the harmonics, but any

periodicity gets geological meaning, if it is supported by geological evidences and considerations, not the other way round. Second, Kitanidis (1997) mentions a couple times the principle of Occam's razor, that is, the use of the simplest empirical model consistent with the observed data. Taking into account how many assumptions the geostatistical approach involves, citing the Occam's razor as one of the reasons for the geostatistical approach sounds at least ironic.

This chapter happened to be much longer than I expected. And the reason is that due to brilliancy of the leading geostatisticians, geostatistics won the market, at least, in terms of scientific publications. I speak without any irony about their brilliancy. They have solved many difficult mathematical problems and obtained many beautiful results. Unfortunately, all this does not resolve the issue of the uncertainty of the results of hydrogeological modeling. The reason for the failure to resolve it is the use of too many assumptions and postulates most of which cannot be tested or are just not true. In the beginning of the application of geostatistics to hydrogeology, they honestly declared that those assumptions and postulate are introduced for convenience only. We do not hear much about it at present. Frequent use and tradition have made them as if valid. It seems that many geostatisticians have believed that geostatistics really overcomes the uncertainty of groundwater modeling problem. They communicate their belief to the community of decision-makers and there exists a great danger if the decision-makers believe them. This reminds me the situation described by known British statistician Kendall (1959) in his poem "Hiawatha Designs an Experiment". Fortunately, pragmatic Indians had enough of sound sense not to believe their famous tribesman Hiawatha, statistician.

On the other hand, if somebody has enough data and wants to use the geostatistical methods as a tool of interpolation and extrapolation of sparse data and does not pretend falsely that this methodology permits evaluating the uncertainty in a provable way, the geostatistical approach is as good or bad as the deterministic one. Although it is more cumbersome, the development of computational technique and methods make this factor less and less significant.

The statistical methods are a powerful instrument for organizing, sorting, analyzing data, revealing whether the data support a hypothesis, or that their structure has peculiarities which may possibly change the comprehension of a site or a phenomenon. They are rather a starting point of developing conceptual geological models. They permit calculating the confidence intervals and many other statistics. But all of them are conditioned by different assumptions. And the more assumptions are introduced, the less must be the trust to the conclusions following from applications of those assumptions.

In general, the situation with the geostatistics is not so bad. Once a proponent of geostatistics asked me why I am against it: "Nobody uses it in practice,"—added he. And this is true. Serious application of geostatistics to hydrogeological problems requires such amount of data that it is not feasible to acquire physically and economically in the most hydrogeological and environmental projects.

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Chapter 4
Model Identification

To predict responses of geological objects on man-made or natural impacts applying mathematical methods, i.e., by solving differential or integral equations, the pertinent properties of the geological objects should be assigned continuously, that is, at each point of the objects and at each instant of the period of simulations, if the properties vary in time, besides maybe countable sets of points, i.e., isolated in space and time points. The boundary and initial conditions must be known in the same way. Unfortunately, only an infinitesimal part of the required geological information is available for direct observations and measurements. The information gap must be filled and geological models do the job. They are a tool of interpolation and extrapolation of the sparse available data on all points of the geological objects of interest.

Geologists, with their understanding of geological surroundings seem to be the best developers of geological models representing geological objects in simulations. But as discussed earlier, those models are not exact copies of real geological objects. The results obtained by using the geological models cannot reproduce simulation processes exactly. So the goal of predictive simulating is to yield the best, in some predefined sense, possible results. To this end the models must be furnished by the values of the model governing parameters providing those results. Such parameters, their values, are called *effective parameters*.

The engineering and geostatistical approaches differ by the ways of assigning the effective parameters. Proponents of the engineering approach just know, from theirs and their colleagues' practical experience, what models and what values of their parameters, which may be some statistics, are best in a given situation. Geostatisticians apply more complicated statistical methods inherent to their general concept. Both approaches test and refine their choices of the effective model parameters observing how they reproduce the available data.

This process of finding or refining predictive model parameters based on available observations on natural or induced hydrogeological phenomena is known as model identification, model calibration, historical matching, and site specific validation. Model identification is often considered as inverse problem solving (Yakowitz and Ducstein 1980; Yeh and Yoon 1981; Carrera and Neuman 1986; Yeh 1986; Hornung 1990; van Genuchten et al. 1990; Aster et al. 2005: Carrera et al. 2005;

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
Springer Hydrogeology, DOI: 10.1007/978-3-319-03569-7_4,

Moore and Doherty 2006; Doherty and Christensen 2011). However, in general, the term 'inverse problem' is not a synonym of the term 'model identification' and its synonyms listed above (see Chap. 9).

Calibration is the most trusted method for assigning the effective parameters of the predictive hydrogeological models at present. The results of calibration are often considered as the strongest argument in support of model's soundness. The faith in the model calibration is based, at least in part, on the belief that the identified parameter values compensate automatically for unknown details. Flavelle (1992) writes: "The calibration (or tuning) of model can be described by a goodness-of-fit parameter which reflects how well the calibrated results match the observed data being simulated. This scalar parameter should incorporate the measurement uncertainty of the observations as well as the uncertainty in the model output." He also holds that "validation tests can also be designed simply to measure the accuracy of the predictions, without reference to a predetermined accuracy as a criterion for acceptance or rejection". The late statement expresses, likely, the Flavelle's belief that we can judge the accuracy of the future simulations based on the accuracy of calibration of predictive models.

Some other professionals, relaying on the model identification as an effective tool, are more cautious. Cited in Chap. 2 De Morsily et al. (1992) emphasize that success in calibration "does not prove that the model will be correct for all circumstances, it only increases our confidence in its value." Indeed, there exist many facts that put in doubt the statements like those of Flavelle (1992). Thus, Yakowitz and Ducstain (1980) describe failures of several successfully calibrated models to predict the hydraulic head development on the same water intake. They explain the failures by incorrectness of the model identification, equating it to the inverse problem. Freyberg (1988), using numerical experiments, demonstrated that success in prediction may not be related to success in matching observed heads and that a good calibration alone may not lead to good prediction.

Based on general philosophical considerations and examples from hydrogeological modeling practice, Konikow and Bredehoeft (1992) claim that a site specific validation "per se, is a futile objective", the point disputed by De Marsily et al. (1992). Beven (1989) goes even further, holding that the use of calibration as a tool for setting model parameters is rather "an act of faith that is not based on sound physical reasoning". Oreskes et al. (1994), state: "Verification and validation of numerical models of natural systems is impossible," and so on.

Accepting the philosophical arguments of Beven (1989); Hornung (1990); Morton (1993); Oreskes et al. (1994); Oreskes (2004), and others that successful model calibration does not guarantee success of predictive simulations, it seems too much to claim that a site specific validation is "a futile objective". We should analyze every piece of available information. Model calibration is one of the tools for such analysis. Playing with different models and parameter values can help with better understanding geology and hydrogeology of the objects and their possible responses on natural or man-made impacts, and why a specifically site-validated model could become misleading in predictive simulations.

4.1 Incorrectness in Mathematics

The usual explanation for model identification to yield misleading results is that it is an ill-posed, incorrect, problem. This makes it worth discussing the mathematical notion of incorrectness in more details.

A problem *is well-posed, correct*, if three following conditions hold:

1. The problem has a solution
2. The solution is unique
3. The solution is stable (continuous), meaning that small errors in the data lead to small errors in the solution

If at least one of the above conditions is violated, the problem is *ill-posed, incorrect*.

One of the main causes of incorrectness is the observation and rounding errors. Their roles could be seen from the following simple example.

Let us consider evaluating of parameter A based on observation of the process described by equation

$$x = A\, e^{-2t} \tag{4.1a}$$

where t and x are the independent and dependent variables. The solution of this inverse problem follows directly from Eq. 4.1a:

$$A = x\, e^{2t} \tag{4.1b}$$

The process described by Eq. 4.1a has asymptote $x = 0$ (Fig. 4.1) which makes the processes with different values of parameter A not distinguishable for large values t. However, using good mathematical software we can evaluate parameter A for very large values t. Thus, for $t = 250$,

$$x = 5e^{-500} = 0.35622882033706 \times 10^{-216} \quad \text{and}$$
$$x = 10e^{-500} = 0.71245764067413 \times 10^{-216}$$

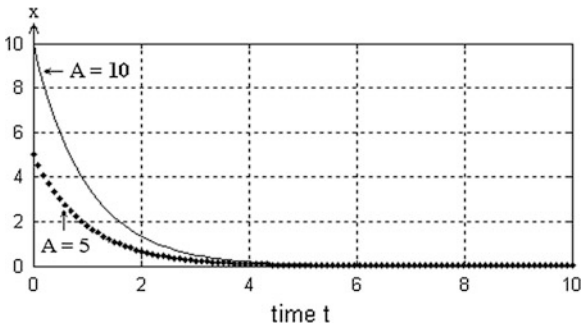

Fig. 4.1 Evaluating parameter A using observations on the process described by Eq. 4.1a

Substituting these values x in Eq. 4.1b yields correspondingly

$$A = 5.00000000000000 \quad \text{and} \quad A = 10.00000000000000,$$

solving our inverse problem more than satisfactorily.

However, as soon as the errors of observations and rounding become commensurable with the observed values, we obtain the situation presented in Fig. 4.1. Assuming that the resolution of the figure corresponds to the accuracy of measurements y, we see that the measurements does not permit separation of the $A = 5$ and $A = 10$ for large enough values t. The problem is correct, say, for $t < 3$ and incorrect for $t > 4$. There exists also a grey zone $3 \leq t \leq 4$ where correctness or incorrectness of the problem depends on the accuracy of the measurements.

This kind of situations is typical for hydrogeological processes developing from transient filtration to steady-state one. Observation and calculation errors can make solving inverse problems impossible for some parameters, if observations are made close to the steady-state phase.

Let the actual behavior of the hydraulic heads be described by function $h(x)$. But what we observe is

$$h_{ob}(x) = h(x) + \varepsilon(x) \tag{4.2}$$

where $\varepsilon(x)$ is the error of the observation at x. In many situations there is a need to evaluate gradient of $h(x)$ based on observations $h_{ob}(x)$. If $\varepsilon(x)$ is not differentiable (a random value, for example), $h_{ob}(x)$ is not differentiable either. So the problem of evaluating the gradient based on observations does not have a solution, it is incorrect.

Now let us assume that the error is differentiable. For example,

$$\varepsilon(x) = A \sin(\omega x) \tag{4.3}$$

where A is the amplitude and ω is the frequency of the oscillations. Then the gradient does exist and can be evaluated as

$$h'_{ob}(x) = h'(x) + A\omega \cos(\omega x) \tag{4.4}$$

The upper boundary for the error in evaluating the gradient of h is $|A\omega|$. If the frequency ω is large, small errors in evaluating x can lead to large errors in evaluating $h'(x)$. This means that the problem of evaluating gradients based on observations can be ill-posed, if even the error is differentiable. We can represent the observations differently, applying different differentiable approximations such as splines, polynomial regressions, and so on. But applying different approximations based on the same observations, we may obtain different gradients.

One-dimensional steady state filtration in a shallow homogeneous unconfined aquifer on the horizontal aquitard in absence of recharge is described by differential equation where $h(x)$ is the thickness of the aquifer, and K is its hydraulic conductivity which is constant:

$$\frac{d\left(K(x)h(x)\frac{dh(x)}{dx}\right)}{dx} = 0 \tag{4.5}$$

If we want to use a homogeneous model ($K(x) = const.$) but the boundary conditions in the model described by Eq. 4.5 are given as the aquifer thickness at the ends of the interval of interest $[0, L]$, we cannot use the model for finding the hydraulic conductivity of the aquifer, since it disappears, is canceled, from Eq. 4.5. This makes incorrect the inverse problem of finding the hydraulic conductivity based on Eq. 4.5. However, let the boundary conditions be known at $x = 0$ as $h(0) = h_0$ and

$$Q(0) = Q_0 = -K(0)h_0\frac{dh(x)}{dx}\bigg|_{x=0} \tag{4.6}$$

Then model presented by Eq. 4.5 can be used for finding the hydraulic conductivity $K(x)$ since

$$\int_0^x \frac{dx}{K(x)} = \frac{h^2(x) - h_0^2}{2Q_0} \tag{4.7}$$

(see Eq. 1.8). In the case of the piecewise homogeneous object with boundaries between its homogeneous parts at points x_i and x_j, the hydraulic conductivity within the those parts could be found as

$$K_{j,i} = \frac{2Q_0\left(x_i - x_j\right)}{h^2\left(x_j\right) - h^2\left(x_i\right)} \tag{4.8}$$

The solution presented by Eq. 4.8 exists for all $h(x_j) \neq h(x_i)$ is unique and stable, since it is continuous with respect to $h(x)$, x and Q_0.

Let us assume that we work with a homogeneous model and have five observations over the thickness of the aquifer. This gives 10 possibilities to calculate the hydraulic conductivity, using Eq. 4.8. If our model, measurements, and calculations are absolutely accurate, then all values of $K_{i,j}$ are the same. But if the model does not reproduce the real object exactly or the measurements and calculations carry errors, it is possible that we can have up to ten considerably different values of the hydraulic conductivity. If the differences between those values exceed what could be expected based on the measurement errors, we have to recognize that our solution becomes not unique and the problem is ill-posed.

There are at least two obvious ways to reformulate the above problem to make it well-posed. One is to accept some statistics of the obtained values $K_{i,j}$ as the solution. On the other hand we can partition the aquifer accordingly to the available observations and than consider that between the observations the aquifer is homogeneous. Then different hydraulic conductivity values characterize different part of the aquifer, so we have a unique and stable solution of our problem

but for the heterogeneous aquifer this time. In both cases we use ad hoc assumptions which usually cannot be verified.

Many inverse and model identification problems are reduced to solving systems of linear equations. Let us start with the following system

$$\begin{aligned} x - y &= 1 \\ x + y &= 3 \end{aligned} \tag{4.9}$$

Matrix of the above system,

$$A = \begin{Bmatrix} 1 & -1 \\ 1 & 1 \end{Bmatrix},$$

can be interpreted as characteristics of a model structure. Its right—hand vector $b = \begin{Bmatrix} 1 \\ 3 \end{Bmatrix}$ can be considered as observed data. The goal is to evaluate parameters x and y which are properties of the model. Note that these parameters being interpreted geometrically are coordinates of the point of intersection of the lines presented by equations of System 4.9.

The problem of evaluating parameters x and y is formulated correctly: it has a unique solution ($x = 2$ and $y = 1$) which is stable. Indeed, let us assume that the structure of the model and the observations carry errors such that instead of System 4.9 we have system

$$\begin{aligned} 0.97x - 1.02y &= 0.99 \\ 1.04x + 0.95y &= 3.02 \end{aligned}$$

The unique solution to this system is $x = 2.03$ and $y = 0.96$. So in response to reasonable inaccuracy of the model and the observations, we have reasonable errors in evaluating parameters x and y.

Let us consider a different system

$$\begin{aligned} x - y &= 1 \\ 2x - 2y &= 3 \end{aligned} \tag{4.10}$$

System 4.10 does not have solution at all: its determinant is equal to zero. Equations 4.10 represent two parallel lines which never intersect. Therefore, the problem of finding parameters x and y System 4.10 is ill-posed.

The system

$$\begin{aligned} 1.05x + 1.05y &= 1.05 \\ 0.98x + 0.98y &= 0.98 \end{aligned} \tag{4.11}$$

has infinity many solutions, since both equations represent the same straight line and any value x and $y = 1 - x$ satisfies System 4.11. Therefore, the problem leading to System 4.11 is ill-posed.

The system

$$\begin{aligned} x + y &= 3 \\ 1.05x + y &= 4 \end{aligned} \tag{4.12}$$

is ill-posed also. Solution of this system is $x = 20$ and $y = -17$. However, if its coefficients carry measurement errors and System 4.12 takes, say, form

$$\begin{aligned} 0.99x + 1.01y &= 3.01 \\ 1.06x + 0.98y &= 3.99 \end{aligned}$$

its solution becomes $x = 10.76$ and $y = -7.56$. Thus small errors in measurements lead to the considerable error in solution. The reason is that the straight lines represented by equations of System 4.13 are about parallel and small errors in their coefficients lead to large errors in the coordinates of their intersection, parameters x and y.

Since systems of linear equations play a considerable part in solving different problems, including hydrogeological ones, let us consider a general system of n linear equations

$$Ax = b \tag{4.13}$$

where A is a square matrix of $n \times n$ size, x is a vector-column of the unknowns and b is a vector-column of the observations (both are of $1 \times n$ size). To have a unique solution, matrix A must have inverse matrix A^{-1}, such that $A^{-1}A = A\,A^{-1} = I$. (I is a unit diagonal matrix: its non-diagonal elements are equal to zero and its diagonal elements are equal to 1.) Matrix A^{-1} exists, if the determinant of matrix A is not equal to zero, $|A| \neq 0$. Then solution to the system can be found by the expression which rather represents a procedure:

$$A^{-1}Ax = x = A^{-1}b \tag{4.14}$$

Discussion on stability of the above solution requires introducing the notion of vector and matrix norms. Let us start with definition of the vector norm.

A *vector norm* $\|a\|$ of vector a is a measure of the vector magnitude. It must be a real number having following properties:

Iv	$\|a\| > 0$	if $a \neq 0$
IIv	$\|a\| = 0$	if $a = 0$
IIIv	$\|\mu a\| = \|\mu\| * \|a\|$	μ is a real number

If b is a vector with norm $\|b\|$ and its dimension is equal to the dimension of vector a, then the following properties hold

IVv	$\|ab\| \leq \|a\| * \|b\|$	Cauchy−Buniakowsky−Schwarz inequality
Vv	$\|a + b\| \leq \|a\| + \|b\|$	Triangle inequality

There exist many different vector norms satisfying the above properties. The most popular vector norms are following:

$$\begin{aligned} \|a\|_1 &= \sum_{i=1}^{n} |a_i| && \text{norm 1} \\ \|a\|_2 &= \left(\sum_{i=1}^{n} a_i^2 \right)^{1/2} && \text{norm or norm 2 or Euclidian norm} \\ \|a\|_\infty &= \max_{1 \le i \le n} |a_i| && \text{norm infinity or maximum norm} \end{aligned} \tag{4.15}$$

Since matrices are sets of vector columns or vector rows, it is natural to associate the matrix norms with the vector ones. Namely for matrix of size $n \times n$ some most often applied norms are defined as

$$\begin{aligned} \|A\|_1 &= \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{j,i}| && \text{norm 1 : the maximum magnitude of sum of matrix columns} \\ \|A\|_F &= \left(\sum_{j=1}^{n} \sum_{i=1}^{n} a_{j,i}^2 \right)^{1/2} && \text{Frobenious norm} \\ \|A\|_\infty &= \max_{1 \le j \le n} \sum_{i=1}^{n} |a_{j,i}| && \text{norm infinity: the maximum magnitude of sum of matrix rows} \end{aligned} \tag{4.16}$$

As an example, let us consider the matrix

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

Corresponding norms are presented in Table 4.1.

The matrix norms have properties of the vector's ones plus one more, related to the matrix–vector product (VIm):

Im	$\|A\| > 0$	if $A \neq 0$
IIm	$\|A\| = 0$	if $A = 0$
IIIm	$\|\mu A\| = \|\mu\| * \|A\|$	μ is a real number
IVm	$\|AB\| \le \|A\| * \|B\|$	Cauchy−Buniakowsky−Schwarz inequality
Vm	$\|A + B\| \le \|A\| + \|B\|$	Triangle inequality
VIm	$\|Ab\| \le \|A\| * \|b\|$	

It is assumed that matrices A and B and vector b in the above list of the properties permit the operations involved. In particular, matrices are assumed to be squared of size $n \times n$.

Table 4.1 Comparing different norms of matrix A

Norm 1	Frobenious norm	Norm infinity
18	16.8819	24

The notion of the coordinated vector and matrix norms permits evaluating errors of the solutions to systems of linear Eq. 4.13. If matrix A and vector b carry errors, then factually System 4.13 becomes

$$(A + \Delta A)(x + \Delta x) = b + \Delta b \tag{4.17}$$

where ΔA is the matrix of errors of the elements of matrix A and Δb is the vector of errors of the elements of vector b and vector Δx is the errors of the elements of vector x. It follows from Eq. 4.17 that

$$\Delta x = A^{-1}(\Delta b - \Delta A\, x - \Delta A \Delta x) \tag{4.18}$$

Applying the norms and the triangle inequality to Eq. 4.18 yields

$$\|\Delta x\| \le \left\|A^{-1}\right\| \times \|\Delta b\| + \left\|A^{-1}\right\| \times \|\Delta A\| \times \|x\| + \left\|A^{-1}\right\| \times \|\Delta A\| \times \|\Delta x\| \tag{4.19}$$

Inequality 4.19 can be reorganized as

$$\frac{\|\Delta x\|}{\|x\|} \le \frac{\lambda}{1 - \lambda \frac{\|\Delta A\|}{\|A\|}} \left(\frac{\|\Delta b\|}{\|b\|} + \frac{\|\Delta A\|}{\|A\|} \right) \tag{4.20}$$

where $\lambda(A) = \|A\|^* \left\|A^{-1}\right\| \ge 1$ is the *condition number*. The condition number $\lambda(A) \ge 1$. Indeed,

$$\left\|A^{-1}A\right\| = \|I\| = 1 \le \left\|A^{-1}\right\|^* \|A\| = \lambda \tag{4.21}$$

Inequality (4.20) relates the relative errors of the solution to System (4.13) and the relative errors of the initial data of matrix A and vector b. The system is *well conditioned*, if $\lambda \approx 1{-}10$. A system is *ill conditioned*, if $\lambda \gg 10^2{-}10^3$. There exists the *gray zone* $10 < \lambda < 10^3$ within which the solution to linear systems may stay stable. Inequality (4.20) is meaningful, if $\lambda \frac{\|\Delta A\|}{\|A\|} \le 1$. This implies that ratio $\frac{\|\Delta A\|}{\|A\|}$ must be considerably smaller than 1. This requirement is practical enough, since there is no sense to work with inaccurate System 4.13.

Note, the notion of incorrectness, as it is formulated in the very beginning of this subsection relates to *mathematical formulations of problems and solutions to them*. It happens sometimes that mathematically correct solution is incorrect physically as, for example, a negative hydraulic conductivity. Why such results may appear and what they mean is discussed in Chaps. 5. However, such situations are easily recognizable and could be rejected or accepted depending on how the physically incorrect solution is intended to be used. (See for more details Chaps. 6–9.) It may also happens, as shown in the following chapters, that a solution looks physically correct but it is incorrect geologically being out of the actual property value range. Such kind of the incorrectness, let us call it

the *geological incorrectness*, is difficult if possible to recognize, though it could lead to catastrophic consequences.

4.2 Regularization of Ill-Posed Problems

The notion of correctness with respect to inverse problem formulations came from the applications of mathematics to studying properties of natural objects. They have unique real property distributions and, if the properties change in time, at each given instant. Their responses on given impacts are a unique also. The responses should depend continuously on small changes of the property values and impacts. Therefore, the inverse problems, using the observed data, must provide those unique distributions of the actual property, impacts and initial and boundary conditions when they are evaluated. (There may be natural processes that are instable inherently. They are not discussed here.)

For these reasons at the time when the existence of the mathematically incorrect problems was discovered, it was natural to think that the incorrectness was caused unfortunate formulations of the pertinent problems. However it later became obvious that there are many meaningful problems that are inherently incorrect. Most problems of geophysical and hydrogeological data interpretation are of this kind. (It is interesting to note that there are no processes in the nature corresponding to inverse problems and model identification in geophysics or hydrogeology.) As soon as this became clear, many methods to treat incorrect problems were developed. Those methods reformulate the incorrect problems in correct ones. Discretization of the hydraulic conductivity and numerical differentiation can be considered as such methods. Indeed, if the locations of the observations $h_{ob}(x_i)$ are such that $x_{i+1} - x_i = x_i - x_{i-1} = \Delta x$, derivative of $h_{ob}(x_i)$ can be evaluated as

$$h'_{ob}(x_i) \approx \frac{h_{ob}(x_{i+1}) - h_{ob}(x_{i-1})}{2\Delta x}.$$

As mentioned above, we can also apply splines, different regressions and many other methods to obtain derivative $h'_{ob}(x_i)$. However attention is required here, as different methods can provide different values of derivative $h'_{ob}(x_i)$ and even evaluate the derivative which does not exist.

One of the most popular and thoroughly developed methods of converting incorrect problems in correct ones is Tikhonov regularization (Tikhonov and Arsenin 1977; Allison 1979; Aster et al. 2005). Applied to inverse problems, it consists of looking for the set of parameters that minimizes the functional

$$\beta = \sum_{j=1}^{m} \sum_{i=1}^{n} \left(h_{ob}(x_i, t_j) - h(x_i, t_j, P)\right)^2 + \lambda \sum_{k=1}^{K} \left(p_k - p_{0,k}\right)^2 \qquad (4.22a)$$

In Eq. 4.22a, $h_{ob}(x_i, t_j)$ is the observed value at the point with coordinate x_i at instant t_j. The simulation results are presented by $h(x, t, P)$, where $P = [p_1, p_2, \ldots p_k, \ldots, p_k]$ is the list (vector) of the parameters governing the simulation process, $P_0 = [p_{01}, p_{02}, \ldots p_{0k}, \ldots, p_{0k}]$ is an a priori guess for the unknown values of parameters P, and λ is a small positive number called the regularization parameter. It is assumed often that $P_0 = 0$, meaning that all parameters in a priory guess are equal to zero. Then Functional 4.22a can be rewritten in the form

$$\beta = \sum_{j=1}^{m} \sum_{i=1}^{n} \left(h_{ob}(x_i, t_j) - h(x_i, t_j, P)\right)^2 + \lambda \sum_{k=1}^{K} p_k^2 \tag{4.22b}$$

Tikhonov regularization is a combination of the least squares regression with penalties for a poor priory guessing. Different forms of the penalizing term are also possible. In particular, it can be constructed to penalize larger values of derivatives of the model $h(x, t, P)$ to provide smoother solutions, so the penalizing term is often called the smoothing term. There exist statistical interpretations of Tikhonov regularization. They require additional assumptions on the statistical characteristics of the observations and the model itself, and are not discussed here.

Regularization substitutes one problem with another. Different regularizations of the same problem make up different problems having different solutions. The sophisticated regularization methods, such as Tikhonov regularization, converge to true solutions if the model subjected to the regularization is true, adequate, and the noise, the random errors in observations and calculations, is the only complicating factor. However, all geological models are knowingly false (Morton 1993; Beven 2005). For example, the numbers of the model parameters and the parameters governing the actual processes are different usually. What regularization means and achieves, if it is applied to false models, is disputable. It may be a proper moment to cite V. N. Tatubalin again (Sect. 3.7): "You look for a scalpel, but with such data as you have, you should rather learn to work with a chopper." He meant geostatistics, but it seems to be true with respect to regularization as well.

4.3 Problem-Dependence of Model Identification

The problem-dependence of model identification means that the results of identification depend on the formulation of the model identification problem. This phenomenon is commonly recognized and often cited (Gorokhovski 1977; Yeh and Yoon 1981; Carrera and Neuman 1986; Kool et al. 1987; Hornung 1990; van Genuchten et al. 1990). Practicing hydrogeologists always knew, for example, that the results of pumping test data interpretation depend on interpretation models, and that it is possible to infer different, sometimes considerably different, hydraulic conductivities and transmissivities based on the same data. What surprises is that the problem-dependence is factually ignored in practical applications and theoretical developments of model identification. Commonly it is referred as some kind

of nuisance along with the recommendation to maintain caution. Thus Yeh and Yoon (1981) write: "In order to obtain physically meaningful parameter estimates, caution must be exercised." Hornung (1990) requires lengthy discussion on the coupled predictive and inverse problem and "a thorough knowledge of the difficulties involved," as if, those discussion and knowledge are enough to overcome the problem-dependence. Batu (2006) citing Mercer and Faust (1981) writes: "Confidence in predictive results must be based on (1) a clear understanding of model limitations; (2) the accuracy of the match with the observed historical behavior; and (3) data reliability knowledge about aquifer characteristics."

Hornung (1990) by the way makes an excellent point, coupling predictive and model identification problems explicitly. Indeed, the goal of model identification is to find the parameters of a geological model, the effective parameters, which reproduce the available observations the best in some predefined sense. When the set of the parameter values is found, it furnishes the same structural geological model to solve the coupled predictive problem. However, predictive problems differ from the corresponding problems of identification nearly always. The differences can include size and shape of the objects, impacts, boundary conditions, and monitoring networks. Often models calibrated under steady-state conditions are applied to predicting transient flows. It happens sometimes that the goals of calibration and prediction are different: a model that is calibrated based on observations on hydraulic heads is applied to finding streamlines that are not observable directly. If a model were an exact copy of the pertinent geological object, than the model identification made once would be effective with respect to any predictive problem related to the object. But models are not exact copies of geological objects, and this causes the problem-dependence. Namely, the effective set of model parameters providing the best prediction of one kind, say, the water table elevations, may not be and often is not the best one for a different kind of predicting, say, the streamlines (Beven 1989; Neuman and Orr 1993; Cooley 2004). Even more, values of the effective parameters can change with the time without any changing in the simulation problem formulation (see Chap. 7).

Let us consider a simple and transparent example (Fig. 4.2): a confined aquifer consisting of two homogeneous bodies: one has the hydraulic transmissivity T_1 and the other T_2. In the initial state the aquifer had the uniform distributions of the hydraulic heads $h(x, 0) = H_0$. At instant $t = 0$, the hydraulic head at $x = 2L$ jumps instantly to $h(2L,\ 0) = H_{2L}$ and then remains unchangeable: $h(2L,\ t) = H_{2L}$. At $x = 0$ the hydraulic head does not change: $h(0,\ t) = H_0$. This jump of the hydraulic head initiates changing the aquifer hydraulic heads. We wish to predict this process using a homogeneous model of the aquifer with the constant effective hydraulic transmissivity $\hat{T}$ which value is to be found.

The simulated process of developing of the hydraulic heads in this case when neither sources nor sinks are present in interval $[0, 2L]$ is described by equation

$$S\frac{\partial \hat{h}(x,t)}{\partial t} = \hat{T}\frac{\partial^2 \hat{h}(x,t)}{\partial x^2} \tag{4.23}$$

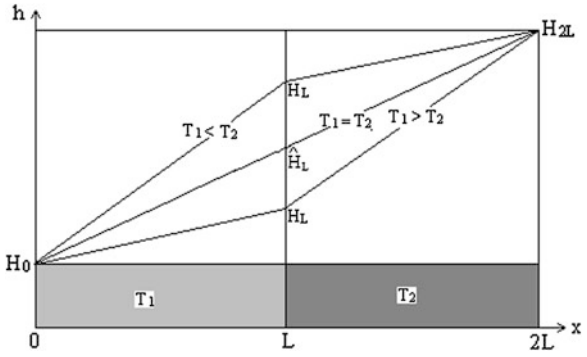

Fig. 4.2 Modeling a confined aquifer with a homogeneous model

where $\hat{h}(x,t)$ are the simulated hydraulic head at point x and instant t, $\hat{T}$ is the effective hydraulic transmissivity of the homogeneous model and S is the known constant storativity. It is assumed also that, observing the process during some not long period of time, the effective value of the model transmissivity $\hat{T}$ is to be found.

To see what will happen to the simulation results with the use of the homogeneous model, let us consider the steady-state distributions of the simulated $\hat{h}(x,\infty)$ and actual $h(x,\infty)$ hydraulic heads, i.e., when the process reaches the steady state. Then the left-hand part of the Eq. 4.23 becomes zero, and the effective transmissivity disappears from the equation, being concealed. Thus, the steady-state distribution of the simulated hydraulic heads is described by equation

$$\frac{d^2\hat{h}}{dx^2} = 0$$

which does not depend on the transmissivity. With the boundary conditions assigned as

$$h(0) = H_0 \quad \text{and} \quad h(2L) = H_{2L} \tag{4.24}$$

the solution to the simulated hydraulic heads $\hat{h}(x,t)$ is

$$\hat{h}(x) = \frac{H_{2L} - H_0}{2L}x + H_0 \tag{4.25}$$

Solution 4.25 corresponds to the straight line (H_0H_{2L}) in Fig. 4.2 with

$$\hat{H}_L = \frac{H_{2L} + H_0}{2} \tag{4.26}$$

The steady-state filtration in the heterogeneous aquifer consisting of two geological bodies with the hydraulic transmissivities T_1 and T_2 is described by two functions: left $h_1(x)$ within interval $[0,\ L]$ and right $h_2(x)$ within interval $[L,\ 2L]$. The functions are solutions of the differential equations

$$\frac{d^2(h_1(x))}{dx^2} = 0 \quad \text{and} \quad \frac{d^2(h_2(x))}{dx^2} = 0 \tag{4.27}$$

under the outer boundary conditions: $h_1(0) = H_0$ and $h_2(2L) = H_{2L}$. There exist also the inner boundary condition on continuity of the hydraulic heads and the flux at $x = L$:

$$h_1(L) = h_2(L) \quad \text{and} \quad T_1 \frac{dh_1(x)}{dx}\bigg|_{x \to L} = T_2 \frac{dh_2(L)}{dx}\bigg|_{L \leftarrow x} \tag{4.28}$$

The conditions connect the solutions of Eq. 4.27 which are

$$h_1(x) = \frac{H_L - H_0}{L} x + H_0, \quad 0 \le x \le L \tag{4.29a}$$

$$h_2(x) = \frac{H_{2L} - H_L}{L} (x - L) + H_L, \quad L \le x \le 2L \tag{4.29b}$$

where the unknown H_L is the same for both solutions (the first Condition 4.28). To find H_L, the condition on continuity of the flux (the second Eq. 4.28) should be applied. Since functions $h_1(x)$ and $h_2(x)$ are straight lines, their derivatives are equal to their slopes. So we can rewrite the second Eq. 4.28 as

$$T_1 \frac{H_L - H_0}{L} = T_2 \frac{H_{2L} - H_L}{L} \tag{4.30}$$

Solving Eq. 4.30 for H_L we obtain

$$H_L = \frac{T_1}{T_1 + T_2} H_0 + \frac{T_2}{T_1 + T_2} H_{2L} \tag{4.31}$$

Thus, the steady-state hydraulic head H_L at the midpoint $x = L$ is an average of H_0 and H_{2L} weighted according to the actual hydraulic transmissivities. The equality $\hat{H}_L = H_L$ is true only if the aquifer is homogeneous ($T_1 = T_2$). If $T_1 > T_2$, then $H_L > \hat{H}_L$, and if $T_1 < T_2$, than $H_L < \hat{H}_L$ (Fig. 4.2). The magnitude and sign of the deviation of $\hat{H}_L$ from the observed value H_L depend on H_{2L} and H_0, the ratio T_2/T_1 and time.

Thus, calibrating the homogeneous model in transient regime can permit the simulation results to fit the observation satisfactory for some period of time. Then the simulated and actual hydraulic heads will start diverging inevitably. If the calibration period is short, we may not see the divergence. But it makes itself known later, in prediction.

The point of this simple example is obvious. The effective parameters of the simplifying models may not and usually do not compensate for the unknown. We cannot evaluate the error of the simulation results yielded by our homogeneous model even in our simple case. It is possible that something like this caused the failures described by Yakowitz and Ducstein (1980). The unlucky simulation models could be the source of failures described by Kola (1984); Lerner (1985);

Kerr (1993) and many others. However, in the presented case the homogenous model can be applied successfully for solving our predictive problem. To this end the effective hydraulic transmissivity must vary in time (see Chap. 7).

4.4 More Complex Model Versus Less Complex One

That all models are false is no news. Practicing hydrogeologists know also that those false models often provide practically acceptable results. Otherwise modeling would not have any sense at all. Nevertheless it seems interesting to illustrate this contradiction (false models and acceptable results) on a simple-real life example. However, our notions on real geological objects are not more than models, and as such they are false. The only option left is to compare the results yielded by a more complex model, considering it, as if, true, and less complex which is false undoubtedly. It is desirable to find a simple and well-studied object to make the comparison simpler.

The Borden landfill (Ontario, Canada) seems appropriate for such an exercise. It was in operation from 1940 to 1976. The contaminant plume in the shallow aquifer below the landfill was the subjected to detailed investigations that lasted from 1974 to 1980. The simplicity of the site as a hydrogeological object, the sharply delineated plume, and relatively large amount of data make the Borden site a suitable object for testing different approaches and models that has been done more than once (Frind et al. 1985; Frind and Hokkanen 1987; Batu 2006).

The more complex model is the model applied by Frind and Hokkanen (1987). They simulated two-dimensional steady-state flow in the Borden aquifer in terms of streamlines. Correspondingly, the boundary conditions are assigned as specific fluxes normal to the object's boundaries. The main goal of their model calibration is to find the specific fluxes on the boundaries of the Borden site aquifer that provide the best reproduction of the observed streamlines. (As discussed below, only one streamline can be considered as observable within the Borden site. Likely, the hydrogeological part of model had been calibrated by reproducing that streamline.) Then they applied the obtained results, the recharge pattern and the streamlines, to simulate contaminant-transport by the Borden aquifer.

The competing model is D1_Flow model developed by US EPA (Gorokhovski and Weaver 2007). It is a screening-level model numerically simulating one-dimensional steady-state flow in shallow unconfined aquifers on an arbitrary shaped base. The model permits evaluating water table, streamlines and time for contaminants to travel to selected locations. Being simple in terms of data preparation and operating, it saves considerable resources and cost. The D1_Flow model is based on the Dupuit-Forchheimer simplification neglecting the vertical component of the Darcy velocity and considering only its horizontal component which simplifies the mathematical description of the underground flow considerably. The D1_Flow model has been validated thoroughly on available, not numerous, analytical solutions for the shallow aquifer on the horizontal and sloppy

(Polubarinova-Kochina 1962) bases. The results are more than satisfactory. The Borden site object has been chosen for validating the D1_Flow model on a real-life object (Gorokhovski and Weaver 2007).

Compared with the more physically sound two-dimensional model by Frind and Hokkanen (1987), the D1_Flow model is undoubtedly false: it simulates one-dimensional flow which is actually at least two-dimensional, uses the knowingly false Dupuit-Forchheimer assumption and the physically controversial method, suggested by Strack (1989) and described in Sect. 4.4.3, for calculating two dimensional streamlines applying based on the results yielded by one-dimensional simulation. Model of Frind and Hokkanen (1987) does not need all these assumptions and simplifications.

The main goal of the D1_Flow model calibration below is to demonstrate that a simple and false model can yield results comparable to the results of more complicated and physically sound models such as that of Frind and Hokkanen (1987). Unfortunately, the factual data used by Frind and Hokkanen (1987) in calibrating their model as well as the accuracy of reproducing by their model the corresponding observations were not available. For this reason, only the results obtained graphically from their publication are used in the D1_ Flow model calibration. A byproduct of the D1_Flow model calibration below is explicit demonstration of the problem-dependence of model identification. Frind and Hokkanen (1987) deal with this phenomenon, though without mentioning it.

4.4.1 Short Description of the Borden Landfill

The unconfined aquifer under the Borden landfill consists of beds and lenses of fine-, medium- and coarse-grained sand overlying an extensive deposit of clay and sandy silt. The 10 ppm outline of chloride is chosen as the boundary of the contamination plume. The longitudinal cross section of the site with the water table, the contaminant plume, and the aquitard surface (Fig. 4.3) is obtained graphically from Frind and Hokkanen (1987). The hydraulic conductivity of the Borden aquifer is assigned based on pumping and permeability tests as equal to 10.11 m/day in the horizontal direction and 5.05 m/day in the vertical direction. (D1_Flow simulations ignore this anisotropy and use only the horizontal hydraulic conductivity 10.11 m/day.)

4.4.2 Simulating the Water Table

Frind and Hokkanen (1987), simulating the contaminant plume development within the Borden site, assume that the flux in the Borden aquifer is steady-state. Their problem formulation requires that the boundary conditions be stable as well as the boundaries themselves. In particular, they assumed that the water table and

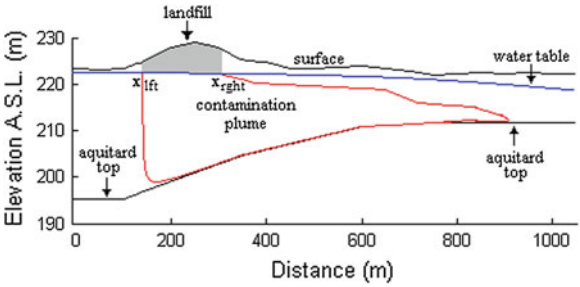

Fig. 4.3 Cross-section of the borden landfill site

precipitations do not change in time. In reality the water table is affected by the seasonal changes of precipitation. Thus, their first task to be addressed is to assign, as if, the long-term average steady-state water table. Frind and Hokkanen (1987) write: "The aspect of the water table has been addressed by Frind et al. (1985)" who in turn resolve the issue by stating: "The water table boundary was obtained visually drawing a smooth curve through the relevant water level points." [By the way, Fig. 15 of Frind et al. (1985) and in Fig. 4 of Frind and Hokkanen (1987) reveal that the water tables used in those works differ by up to 0.6 m.] The "relevant points" are the factual observations in April and December 1979. The water table such assigned is arbitrary in essence. Besides it is biased with respect to the available observations (Fig. 4.4). However, it is likely, that the water table was just an intermediate and not decisive part of their calibration processes. Their final goal was "matching streamlines to the observed plume" (Frind et al. 1985).

The D1_Flow model is calibrated with respect to the water table of Frind and Hokkanen (1987). The goal is to reproduce their water table by varying piecewise constant recharge rates within the recharge pattern structure presented by Frind and Hokkanen (1987). The boundary conditions is assigned in the water divide at $x = 135$ m where the water table elevation is 222.36 m and the total flux Q is consequently zero. The choice of the boundary conditions is based on the figures of Frind and Hokkanen (1987). It supported by their boundary conditions. Indeed, the specific flux on the boundary at $x = 0$, where thickness of the aquifer is about 30 m, is assigned as -70 cm/year. The recharge rate in interval [0, 140] m is assigned equal to 15 cm/year. The water table divide seems to be somewhere close but not exceeding 140 m, since there is no evidence of a contaminant up-gradient to the landfill. The recharge pattern provided by simple D1_Flow model (Table 4.2 reproduces the water table by Frind and Hokkanen (1987) with the error magnitude less than 5 cm (Fig. 4.4), i.e., satisfactory.

It is interestingly to note that if 1979 was not a special year with respect to the long-term precipitation regime for the Borden site, it could be reasonable to present the long-term steady-state water table as some averaging of the observations in April and December. The least squares method applied to those observations yields the following regression equation for depicting the water table:

$$r\hat{H}(x) = -2.5725 \times 10^{-6}x^2 - 7.7991 \times 10^{-4}x + 222.5731 \text{ m} \qquad (4.32)$$

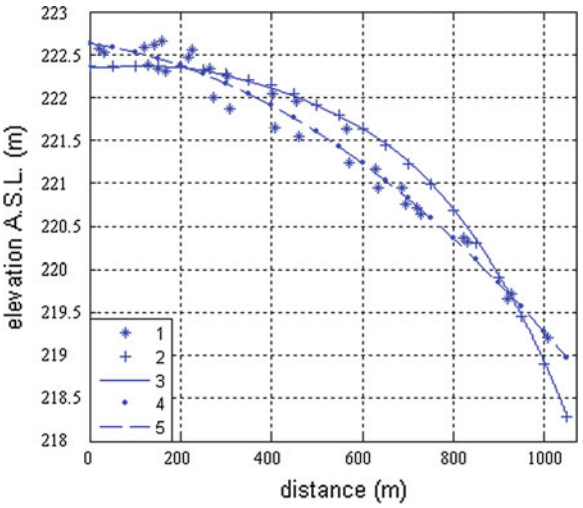

Fig. 4.4 Observed, assigned and calibrated water tables: *1* observations, *2* water table assigned by Frind and Hokkanen (1987), *3* reproduction of the water table of Frind and Hokkanen (1987) by D1_Flow model, *4* water table approximated by regression 4.32, *5* reproduction of regression 4.32 by D1_Flow model

Table 4.2 Recharge patterns according to Frind and Hokkanen (1987) and D1_Flow model (cm/year)

Interval (m)	0–140	140–300	300–600	600–800	800–1050
Frind and Hokkanen (1987)	15	55	15	45	10
D1_Flow model	15	55	10	50	12

Table 4.3 Recharge pattern calculated by Eq. 4.33 (cm/year)

Interval (m)	0–140	140–300	300–600	600–800	800–1050
Equation 4.3	34	9	−1.6	2.7	−10

(Other regression presentations of the water table are possible also.) The water table described by Eq. 4.32 is presented in Fig. 4.4. The corresponding total flux is described by equation

$$r\hat{Q}(x) = K\frac{d(rH)}{dx}(rH(x) - Y(x)) = K\left(5.145 \times 10^{-6}x + 7.7991 \times 10^{-4}\right)(rH(x) - Y(x))\ \mathrm{m}^2/\mathrm{day} \quad (4.33)$$

where K(m/day) is the hydraulic conductivity and $Y(x)$ is the aquifer base elevation (m). The water table simulated by the D1_Flow model and based on the piecewise recharge rate calculated by Eq. 4.33 (Table 4.3) reproduces the water table depicted by Eq. 4.32 with the error magnitude less than 4 cm. Interestingly that Frind et al. (1985), obtained negative recharge rate, −30 cm/year for x greater then 700 m, though the '*slightly modified*' recharge pattern of Frind and Hokkanen (1987) does not contain negative recharge rates (Table 4.2).

Note, the assumption about the existence of the water divide in the long-term average steady-state flow system makes the flow in the Borden aquifer three-dimensional. It could be considered two-dimensional along the axis of symmetry, if such axis exists. Likely, Frind et al. (1985) and Frind and Hokkanen 1987, assume this implicitly.

Two observations above are just digressions. Since the goal is to demonstrate that the simple, and false, model D1_Flow is able to reproduce the results obtained by the complex model of Frind and Hokkanen (1987) we continue working with the data used and obtained in process of calibration by Frind and Hokkanen (1987).

4.4.3 Calibration with Respect to the Streamlines and the Arrival Time

As mentioned above, Frind and Hokkanen (1987), following to Frind et al. (1985), assigned their water tables arbitrary and then calibrated the flow system based on the plume configuration "matching streamlines to the observed plume" (Frind et al. 1985). There are only two streamlines which could be considered, as if, observed: the upper and bottom boundaries of the plume. The bottom boundary is not informative, since the corresponding streamline starts nearby the water divide and seepage along this streamline is extremely low, theoretically equal to zero. Thus only the sharply outlined upper boundary of the Borden plume can be interpreted as the streamline to be used in calibration.

Calibrating their model with respect to the streamlines Frind and Hokkanen (1987) following Frind et al. (1985), scale simultaneously the recharge rates and the hydraulic conductivity. Such scaling does not change the structure of the flow simulated by their model. However, the hydraulic conductivity of the Borden aquifer is evaluated based on pumping and permeability tests. As such, it must be considered as an objective characteristic of the Borden aquifer. Scaling the hydraulic conductivity is ad hoc substituting one geological object with another. Since the recharge pattern is not observable and is evaluated as an effective characteristic, it seems more natural to manipulate the recharge rates only. Frind and Hokkanen (1987) do not explain their reasons for the scaling. Likely, they did this to satisfy the travel time to reach the furthest location to which the plume has been spread somewhere 600–650 m from the down-gradient edge of the landfill. Proportional decreasing the recharge rates and the hydraulic conductivities increases the travel time.

At first sight, the Dupuit-Forchheimer simplification ignoring the vertical component of flow does not have tools for simulating curved, two-dimensional, streamlines. Strack (1989) overcomes this controversy, suggesting that the incoming recharge pushes down the existing streamlines, curving them. He provides the mathematical expression describing the process. Gorokhovski and Weaver (2007), developing the D1_Flow model, applied his approach to one-

dimensional flow in horizontally heterogeneous aquifers on the arbitrary shaped base.

Let streamline S originate at location x_{st} on the water table (Fig. 4.5) and Q_S denotes the total flux $Q(x)$ at $x_{st}(Q_S = Q(x_{st}))$. Streamline S is the upper boundary of the Q_S part of the total flux $Q(x)$. Since the specific flux does not depend on depth according to the Dupuit-Forchheimer simplification, the following equality holds at any location $x \geq x_{st}$:

$$\frac{Q(x)}{Q_S} = \frac{H(x) - Y(x)}{H_S(x) - Y(x)} \tag{4.34}$$

where $H(x)$, $H_S(x)$, $Y(x)$, and $Q(x)$ are the elevations of the water table, streamline and aquifer base and the total flux; index S relates to the streamline $S(Q_S = Q(x_{st}))$. It follows from Eq. 4.34 that

$$H(x) - Y(x) = \frac{Q(x)}{Q_S}(H_S(x) - Y(x)) \tag{4.35}$$

The travel time for a particle to reach location x moving along streamline S is

$$t(x) = R\theta \int_{s_{st}}^{s_x} \frac{ds}{v(s)} \tag{4.36}$$

where R is the retardation factor, θ is the effective porosity and $v(s)$ is projection the horizontal Darcy velocity $v(x)$ on streamline S. (According to Frind and Hokkanen 1987, for the Borden aquifer, $\theta = 0.38$ and $R = 1$.) In one-dimensional filtration model the Darcy velocity at any location x can be presented as

$$v(x) = \frac{Q_S}{H_S(x) - Y(x)} \tag{4.37}$$

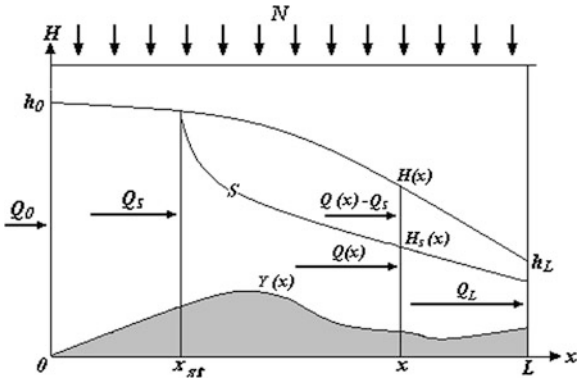

Fig. 4.5 Streamline calculation: $H(x)$, $H_S(x)$, $Y(x)$, and $Q(x)$ are the elevations of the water table, streamline and aquifer base and the total flux at location x, $N(x)$ is the recharge, S is the streamline $(Q_S = Q(x_{st}))$

Correspondingly

$$v_S(x) = \frac{v(x)}{\sqrt{1 + \left(\frac{dH_S(x)}{dx}\right)^2}} \tag{4.38}$$

and Eq. 4.36 can be rewritten as

$$t(x) = \frac{R\theta}{Q_S} \int_{x_{st}}^{x} (H_S(x) - Y(x)) \left(1 + \left(\frac{dH_S(x)}{dx}\right)^2\right) dx \tag{4.39}$$

The D1_Flow model integrates Eq. 4.39 numerically, using the Trapezoid rule.

The D1_Flow model has been calibrated with respect to the upper boundary of the plume representing the streamline starting at the water table beneath the down-gradient edge of the landfill at $x = 300$ m. This streamline is the shortest and fastest way for contamination to spread. The goal of the calibration is evaluating of the recharge pattern for $x > 300$ m which provides the best reproduction of the streamline and the travel time for the plume to reach the furthest distance from the landfill which is located somewhere in interval 900–950 m. The starting point of calibrating is the recharge pattern accepted by Frind and Hokkanen (1987) (Table 4.4).

Calibration has been conducted in two steps. First, the recharge pattern was found providing the best reproduction of the streamline. The results are presented in Table 4.4 and Fig. 4.6. Magnitude of the errors in the best reproduction of the streamline by D1_Flow model is equal to 5 cm. The second step is necessary, since the travel time for the contaminant to reach $x = 900$ m along the obtained streamline and the recharge rates is about 32 years instead of expected 39–40 years. The recharge pattern providing the travel time equal 39.1 years to $x = 900$ m and 40.2 years to $x = 950$ m presented in Table 4.4 also. The total flux Q_S under this streamline is 0.1253 m/day. It seems to be satisfactory compromise between reproducing the shape of the stream line and the available travel time. Magnitude of the errors in reproducing the observed streamline is less than 5.04 cm. Some other streamlines obtained by of Frind and Hokkanen (1987) and the D1_Flow model are shown in Fig. 4.7.

The calibration procedure has been simplified by the fact that according to Eq. 4.34 the simulation results are defined by the ratio Q/Q_S. However since the model is not exact copy of the geological object and the procedure utilized in the D1_Flow model is not more than the approximation of the real process, the final

Table 4.4 Recharge patterns (cm/year) for evaluating streamlines and travel time

Interval (m)	0–140	140–300	300–600	600–800	800–1050
Frind and Hokkanen (1987)	10	37	10	30	7
D1_Flow model:					
Best streamline	7	34	12.1	26.5	10
Best travel time	5.85	28.41	10.2	23	8.36

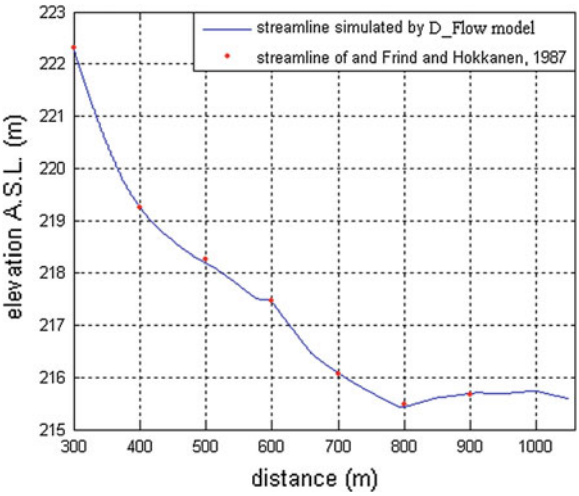

Fig. 4.6 Results of calibration of the D1_Flow model based on data of Frind and Hokkanen (1987) on the streamlinestarting at $x = 300$ m

part of the second step required manual fitting the simulation results to the observations. The manual fitting is not cumbersome either: D1_Flow model permits fitting the available data sequentially.

Summarizing, the simple D1_Flow model exploiting some obviously false assumptions yields the results which are practically comparable to those yielded by the more physically sound model of Frind and Hokkanen (1987). In principle, models with the larger number of governing parameters are more flexible: they are easier to fit the available observations. For example, the D1_Flow model, simulating the Borden plume, could reproduce the observation absolutely accurately, if

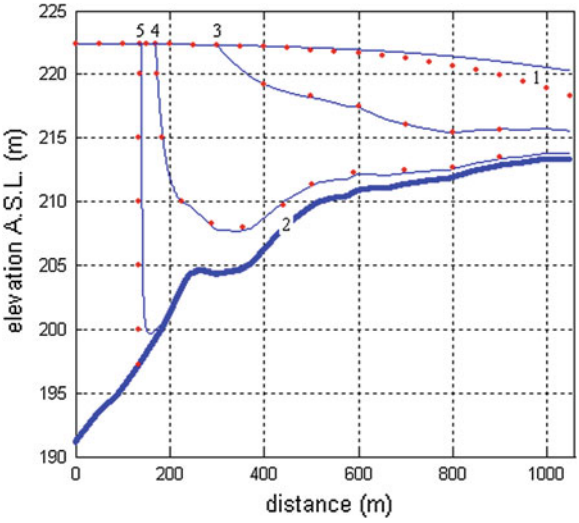

Fig. 4.7 Results of calibration of the D1_Flow model (*solid lines*) with respect to streamlines of and Frind and Hokkanen (1987), (*dots*): *1* water tables, *2* base of aquifer, *3* streamline starting at $x = 300$ m, *4* streamline starting at $x = 170$ m, *5* streamline starting at 140 m

the recharge rates had changed at the points (stayed constant between the points) of observations. But what does this prove? Thus, the quality of calibration, fitting the available observations, cannot be a decisive reason for choosing a model. (Compare with the chose of mathematical expressions depicting regional trends discussed in Sect. 3.1 and illustrated by Fig. 3.1.)

The calibration of both models explicitly demonstrates the problem-dependence of model identification. Indeed, Frind and Hokkanen (1987) scaled the recharge pattern and the hydraulic conductivities to satisfy the factual travel time. Their scaling leads to substituting of the empirically established properties of the object by different model parameters, that is, one object is substituted with another. In the case of the D1_Flow model, to achieve a good fit, the recharge pattern have been manipulated only. The hydraulic conductivity, that is, the hydrogeological object *per se* remained the same. Nevertheless both calibrations can be considered as successful. But the uncertainty of the simulation results in both cases cannot be evaluated in a provable way, since the simulations use many unverified and even incorrect assumption. The most obvious of them is assumptions about steady-state filtrations plus the Dupuit-Forchheimer assumption in the case of the D1_Flow model.

Geological models are not exact copies of the real, not known in full, geological objects which they represent. Those models can be tuned to simulate satisfactorily the problems under conditions imposed in calibration. However, if the conditions change, the parts of the objects, which are unknown, not represented or misrepresented, can affect the objects' responses in the ways which differ considerably from what are expected from simulation models. Namely this causes the problem-dependence of model identification. (Inaccuracy of mathematical model can produce similar effects which might be a subject of special research.)

Model identification in hydrogeology is considered often as an inverse problem. This is not accurate. Model identification is an optimization problem usually. Its solution depends on the systems to be optimized. The systems include a number of factors: structures and properties of the objects, known and not known; the models representing them in simulation; mathematical descriptions of the processes in model; actual and modeled boundary conditions; man-made and natural impacts affecting the available data; criteria of quality of fitting the data; the monitoring networks used for evaluating the criteria. (The list is not exhaustive.) The optimal parameters are optimal, effective, in the sense they are assigned to be effective. However, if the system that they optimize is changed, those effective parameters may loose effectiveness and even become misleading. And this is indeed the case, since predictive problems differ from model identification problems in many respects.

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Chapter 5
Transformation of Geological Objects' Properties into Effective Model Parameters

This short chapter is the key chapter of this book. The preceding chapters demonstrate why successful calibration of hydrogeological models does not warrant success of the simulations based on calibration results and that it is impossible to estimate the uncertainty of the results of hydrogeological modeling, besides the cases where statistics exists on successes and failures of the projects based on the results of hydrological simulation, i.e., in the cases of typical projects in typical geological surroundings. This leaves us with the only option: "to do the best one can with what is available" (US EPA, 1987). One of many possible, I hope, ways "to do the best" is suggested in the following chapters of this book and is based on the concept of transforming mechanisms introduced in this chapter. The mechanisms use the phenomenon of the problem dependence of model identifications and permit obtaining the model parameters which are effective beyond calibration.

5.1 Geological Objects and Simulation Models

As discussed in the previous chapters, to simulate underground flow and mass transport by solving differential equations describing the simulation processes within a site, we need to assign pertinent boundary conditions on the boundaries of the site of interest. Although some of the conditions can be controlled or induced by us, i.e., known, the considerable part of them remains unknown but just assumed. To find the boundaries on which boundary conditions can be established, we usually have to go out of the site of interest. If we cannot find them close enough to our site, then we consider that the boundaries are in infinity and, based on this assumption, evaluate the boundary conditions as close to the site as possible. Thus, simulation models must usually represent larger geological surroundings than the sites of interest.

Let us assume that the goal of simulation is to predict how construction of a landfill can affect water supplying wells (Fig. 5.1). Let rivers 1 and 2 and a channel be closely connected to the aquifer used for the water supply. This permits assignation of boundary conditions along those rivers and the channel and solving the mass transport problem within the territory outlined by the rivers and the channel.

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Springer Hydrogeology, DOI: 10.1007/978-3-319-03569-7_5,

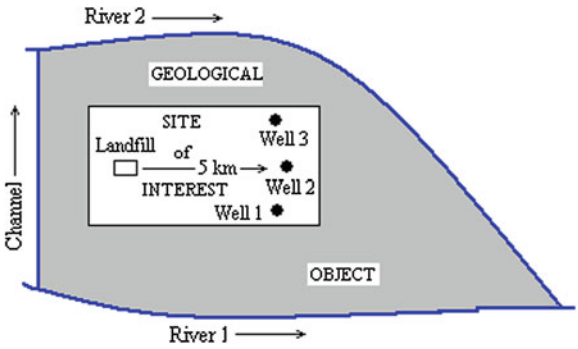

Fig. 5.1 Site of interest and geological object

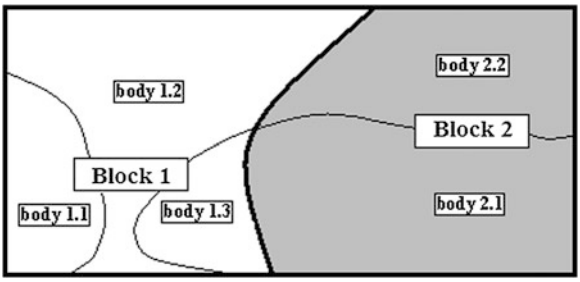

Fig. 5.2 Five body geological structure and two block model

The territory including the sites of interest and outlined by the boundaries permitting assignation of boundary conditions required for solving pertinent hydrogeological and mass transport problems are called here *geological objects* or just *objects*. Homogeneous geological units, the units comprising rocks and soils of the same lithological composition, origin and geological history, are called *geological bodies* or just *bodies*. Their properties are traditionally considered as constant. Space and time trends of the properties are rarely taking in account. But when they are, the coefficients of the corresponding trends can be considered as properties of the geological bodies, constant within them.

Geological models or just *models* are simplified replicas of the geological objects. They introduce rules of interpolation and extrapolation of sparse available data on geological properties at every point of the objects, thereby filling the information gaps created by the paucity of the data. The extrapolation rules are primitive. Models usually consist of homogeneous units called *model blocks* (or just *blocks*): One parameter value of each relevant property substitutes for the variety of that actual property's values within a given model block. This parameter and its value are called the *model block parameter* (or just *parameter*). Figure 5.2 illustrates the notions of the geological object and geological model. The object consists of five geological bodies and the model of two blocks. If bodies 1.3 and 2.1 are actually the same geological body, they are considered as two different bodies, since they belong to different model blocks.

5.2 Transforming Mechanisms

Let an object comprise N geological bodies. Its geological model consists of M blocks ($M \leq N$). Block j represents N_j geological bodies with actual values of property G $(g_{j,1}, \ldots, g_{j,N_j})$, and model block parameter $\hat{g}_j$ substitutes for these values in predictive simulations. Conversion of actual property values of the geological bodies into the effective model block parameter is called the *transformation*. The term is to emphasize that the conversion is not necessarily statistical averaging which is characterized by not negative and summing to one weighting factors.

Since geological models are not exact copies of the geological objects, the simulation results do not reproduce the objects' responses on natural and man-made impacts exactly. We can request only that the results would be best in some predefined sense, i.e., satisfy some criterion of quality on a given monitoring network. The most popular and mathematically convenient is the least squares criterion requiring minimization of the squared residuals between the data observed at the monitoring network and the corresponding simulation results. Other criteria can be applied as well. Model identification is the search for the set of model parameters providing the best, in a predefined sense, results of the pertinent predictive simulation, not just in calibration. Thus, the problem of model identification is an optimization problem.

The model which is best in a defined sense is called *effective*. The corresponding set of its parameters $(\hat{g}_1, \ldots, \hat{g}_j, \ldots, \hat{g}_M)$ is *effective*. Each parameter of the set is the *effective parameter*. A mathematical expression describing transforming actual values of property G of the geological bodies comprising the geological object into the effective parameter $\hat{g}_j$, generalizing property G in block j, is called the *transforming mechanism* (or just the *mechanism*). The following equation represents one of possible forms of such expressions:

$$\hat{g}_j = \sum_{m=1}^{M} \sum_{n=1}^{N_m} w_{j,m,n} g_{m,n} \tag{5.1a}$$

where geological bodies enumerated within each model block: $g_{m,n}$ is the actual value of property G in geological body n ($n = 1$ to N_m) belonging to the model block m, $w_{j,m,n}$ is the affecting factor describing the contribution of the body n belonging to the block m in forming the effective parameter value $\hat{g}_j$ of property G for the block j. Equation 5.1a can be written also as

$$\hat{g}_j = \sum_{n=1}^{N} w_{j,n} g_n \tag{5.1b}$$

where the enumeration of the geological bodies is total ($1 \leq n \leq N$) so g_n and $w_{j,n}$ are the actual value of property G in body n of the object. Block j for which the effective parameter value $\hat{g}_j$ is evaluated is called the *evaluated* block. Other blocks are called *affecting*.

Contrary to statistical averaging, including only the bodies belonging to the evaluated block j, summations in Eq. 5.1a, b include all geological bodies of the geological object. Subsurface flow, as well as mass transport, is a dynamic process affected by the internal conditions on continuity of flow and hydraulic heads or water table elevations at the geological body contacts. The internal conditions bind all geologic bodies of the object in a united system, and the response occurring in a part of the object represented by some model block depends not only on properties of the bodies represented by this block but on properties of each body of the object. Therefore, any transformation of a spatially variable property G related to modeling dynamic processes should incorporate relevant property values of all geological bodies.

Equation 5.1a, b represent a *linear transforming mechanism*, if the affecting factors depend on positions of the geologic bodies and/or time only. Equation 5.1a, b represent a *non-linear transforming mechanism*, if the affecting factors depend on geologic bodies' property values.

The transforming mechanisms can be *property interrelating* also. The interrelation can reflect real bounds as in the cases of the aquifer transmissivity (product of the aquifer thickness and the hydraulic conductivity) and hydraulic diffusivity (quotient of the hydraulic transmissivity and the storativity). The subsurface flow transport models are essentially governed by non-dimensional coefficients, binding different physical parameters. For example, one dimensional steady-state flow in a homogeneous aquifer is described by equation

$$\frac{d\left(h(x)\frac{dh(x)}{dx}\right)}{dx} = -W \tag{5.2}$$

where $h(x)$ is the aquifer thickness and $W = N/K$ where K is the hydraulic conductivity, and N is the recharge. Thus, although Eq. 5.2 includes two parameters, factually it is governed by their dimensionless ratio. In the case of the interrelating mechanisms, the transforming mechanisms presented by Eq. 5.1b take the following form:

$$\hat{g}_{j,s} = \sum_{n=1}^{N}\sum_{p=1}^{P} w_{j,n,p} g_{n,p} \tag{5.3}$$

where $\hat{g}_{j,s}$ is the effective value of property G_s in model block j, and $g_{n,p}$ is the actual value of property G_p of geological body n. The interrelating mechanisms are not discussed in this work, since this would complicate presentation of the concept of the transforming mechanisms.

5.3 Properties of Transforming Mechanisms

Let a geological model be an exact replica of a geological object with respect to property G. This means that each model block is homogeneous in property G; i.e., all geological bodies represented by each block have the same value of

property G. Thus, all bodies belonging to model block m have the same value g_m of property G. It is reasonable to assume in this case that the effective value $\hat{g}_j$ provided by Eq. 5.1a should be equal to the actual value of property in block j:

$$\hat{g}_j = \sum_{m=1}^{M} \left(\sum_{n=1}^{N_m} w_{j,m,n} \right) g_m = g_j \tag{5.4}$$

For Eq. 5.4 to be true for any set $\{g_m\}$ of actual property values, three obvious properties of the transforming mechanisms must hold.

Property 1 *is expressed by the equality:*

$$\sum_{n=1}^{N_j} w_{j,j,n} = 1 \quad \text{for evaluated block } j \tag{5.5}$$

that is, the affecting factors related to the evaluated block j are summing to one in any transforming mechanism forming effective parameter $\hat{g}_j$.

Property 2 *is expressed by the equality:*

$$\sum_{n=1}^{N_m} w_{j,m,n} = 0 \quad \text{for affecting block } m \ (m \neq j) \tag{5.6}$$

that is, the affecting factors for any affecting block are summing to zero.

One more property follows from Properties 1 and 2:

Property 3

$$\sum_{n=1}^{N} w_{j,n} = 1 \tag{5.7}$$

that is, the total sum of all affecting factors is equal to one.

The following example illustrates the above properties of the transforming mechanisms. Let a geological object comprise five geological bodies, and its model consists of two blocks (Fig. 5.3). Two effective parameters ($\hat{g}_1$ and $\hat{g}_2$) must represent actual values of property G in simulations. Two transforming mechanisms convert properties of the geological bodies in the effective model parameters:

$$\begin{aligned} \hat{g}_1 &= w_{1,1}g_1 + w_{1,2}g_2 + w_{1,3}g_3 + w_{1,4}g_4 + w_{1,5}g_5 \\ \hat{g}_2 &= w_{2,1}g_1 + w_{2,2}g_2 + w_{2,3}g_3 + w_{2,4}g_4 + w_{2,5}g_5 \end{aligned} \tag{5.8}$$

where $g_1 = g_{1,1}$, $g_2 = g_{1,2}$, $g_3 = g_{1,3}$, $g_4 = g_{2,1}$, $g_5 = g_{2,2}$ in Fig. 5.3.

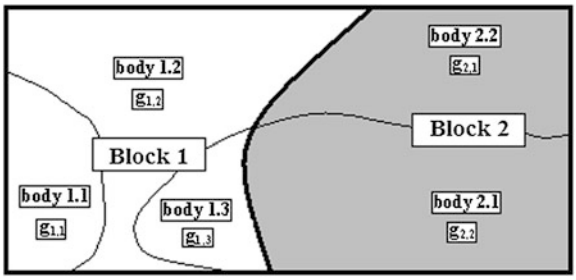

Fig. 5.3 Five-body object and two-block model

Properties of the transforming mechanisms can be easily demonstrated by Mechanisms 5.8. Indeed, let the discussed model be an exact replica of the object. This means that property G is the same within each model block:

$$g_1 = g_2 = g_3 = G_1 \quad \text{and} \quad g_4 = g_5 = G_2. \tag{5.9}$$

Then Eq. 5.8 converts into equations

$$\begin{aligned} \hat{g}_1 &= \left(w_{1,1} + w_{1,2} + w_{1,3}\right)G_1 + \left(w_{1,4} + w_{1,5}\right)G_2 \\ \hat{g}_2 &= \left(w_{2,1} + w_{2,2} + w_{2,3}\right)G_1 + \left(w_{2,4} + w_{2,5}\right)G_2. \end{aligned} \tag{5.10}$$

For the model which is an exact replica of an object, the model block effective parameters are equal to the actual property values:

$$\begin{aligned} \hat{g}_1 &= \left(w_{1,1} + w_{1,2} + w_{1,3}\right)g_1 + \left(w_{1,4} + w_{1,5}\right)g_2 = G_1 \\ \hat{g}_2 &= \left(w_{2,1} + w_{2,2} + w_{2,3}\right)g_1 + \left(w_{2,4} + w_{2,5}\right)g_2 = G_2. \end{aligned} \tag{5.11}$$

Equation 5.11 must hold for any values g_1 and g_2. To make this possible, Mechanisms 5.11 should have Properties 1 and 2:

$$\begin{aligned} w_{1,1} + w_{1,2} + w_{1,3} &= 1 \quad \text{Property 1} \\ w_{1,4} + w_{1,5} &= 0 \quad \text{Property 2} \\ w_{2,1} + w_{2,2} + w_{2,3} &= 0 \quad \text{Property 2} \\ w_{2,4} + w_{2,5} &= 1 \quad \text{Property 1} \end{aligned}$$

It follows from Property 2 that if an affecting block represents more than one geological body, at least one of affecting factors of the block is negative. This means that, in general, the effective parameters of models are not of the statistical nature. That is, they are not statistical averages with the non-negative weighting factors summing to one. In the case of the homogeneous models due Property 1, the effective parameters can be the statistical averages. However, as shown in Chap. 7, summing of the affecting factors of the evaluated blocks to one does not warrant that all the factors are not negative. The fact that all geological bodies of the object participate in forming effective parameters for any block undermines the statistical nature of the effective parameters also.

The effective parameters are the characteristics optimizing the system made up by the geological structure of the object, the model representing it, the boundary conditions, the natural or man-made impact which is to be simulated, the criterion of quality of planning predictive simulations and the monitoring network on which the given criterion is evaluated. The system changes if any of the above listed factors change, and this changes the transforming mechanisms. Even the progress of time can change the transforming mechanisms and the effective parameter values. (See examples in Chaps. 6 and 7.)

The presence of the negative affecting factors in the transforming mechanisms can lead to physically incorrect values of the effective parameters such as negative hydraulic conductivities and transmissivities (see 8). This emphasizes that the effective parameters are deprived of physical meaning. They are system characteristics providing the system efficiency and nothing more. To be effectively in a changed system, different effective parameters and different transforming mechanisms are required (showing problem dependence at work).

A physical incorrect effective parameter is self-obvious. But the effective parameters, being correct physically, may be incorrect geologically, exceeding the range of the actual values of the property they represent. The geological incorrectness is not obvious. The geologically incorrect effective parameters, being effective in a given predictive problem formulation, may become misleading and even dangerous in other applications.

The problem dependence are seen usually as an obstacle or, at least, as a nuisance. On the other hand, the problem dependence of the effective parameters permits obtaining different values of the effective parameters, using different model identification problem formulations. This, in turn, permits better understanding of the structures of geological objects and can be used for formulating and solving inverse hydrogeological problems (Chap. 9). (The transforming mechanisms related to evaluating effective degradation rates are discussed in Chap. 10.)

The transforming mechanisms, defined by their affecting factors, describe contributions of different objects' parts to the effective parameters of the simulation models. Therefore being evaluated before starting field investigations (Chap. 8), they can be a tool for optimization of those. The transforming mechanisms can be applied also for assigning monitoring networks and even simulation models.

The transforming mechanisms are introduced here in the hydrogeological context. However, their introduction does not assume any hydrogeological specificity. It would not be surprising if such mechanisms with the analogous properties are known to professionals in the field of optimization. In any case the transforming mechanisms and their properties can be applied to other fields where simplified versions of complex systems are in use, such as geophysics, engineering geology, environmental sciences.

Chapter 6
Examples of Linear Transforming Mechanisms

In the previous chapter the existence of the transforming mechanisms has been postulated. Their properties follow from their existence and from a natural, but nevertheless, assumption. This chapter contains several simple filtration problems, permitting direct, analytical, inference of linear transforming mechanisms. Mathematically they can be considered as a proof of the theorem of their existence.

6.1 One-Dimensional Steady-State Filtration to Fully Penetrating Trench

Let us consider one-dimensional steady-state underground flow in unconfined aquifer on a horizontal base with constant recharge N to a fully penetrating trench at $X_0 = 0$ (Fig. 6.1). The aquifer is piecewise homogeneous. Its hydraulic conductivity changes at locations X_1, X_2 and X_3, taking within intervals $[X_0, X_1]$, $(X_1, X_2]$, $(X_2, X_3]$, $(X_3, X_4]$ values K_1, K_2 and K_3 and K_4. Recharge $N = 0.0001$ m/day and $X_1 = 25$, $X_2 = 50$, $X_3 = 75$ and $X_4 = 100$ m. The outer boundary conditions are given as the aquifer thickness h_0 at X_0 and the slope (gradient) of the water table at X_4:

$$h_0 = h(X_0), \quad \left.\frac{dh}{dx}\right|_{x=X_4} = 0.$$

Within the homogeneous interval j, $[X_{j-1}, X_j]$, the flow is described by equation:

$$\frac{d\left(K_j\left(h(x)\frac{dh(x)}{dx}\right)\right)}{dx} = -N, \quad X_{j-1} \le x \le X_j \tag{6.1}$$

where $h(x)$ is the aquifer thickness at x.

The inner boundary conditions on continuity of the water table elevation and the flux at locations $X_1 = 25$, $X_2 = 50$, and $X_3 = 75$ m are

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*, Springer Hydrogeology, DOI: 10.1007/978-3-319-03569-7_6,

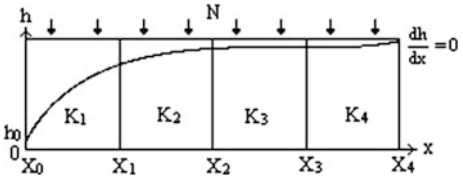

Fig. 6.1 One-dimensional steady-state flow to a fully-penetrating trench in an unconfined aquifer

$$\begin{aligned} \lim_{x \to X_j} (h(x)) &= \lim_{X_j \leftarrow x} (h(x)) \\ K_j \left(h \frac{dh}{dx} \right) \Big|_{x \to X_j} &= K_{j+1} \left(h \frac{dh}{dx} \right) \Big|_{X_j \leftarrow x} \end{aligned} \tag{6.2}$$

Integrating Eq. 6.1, using the boundary conditions for interval $[X_{j-1}, X_j]$, yields (see the inference in the text block 6.1 below):

$$h^2(x) = h_{j-1}^2 + 2\frac{N}{K_j}(L - X_{j-1})(x - X_{j-1}) - \frac{N}{K_j}(x - X_{j-1})^2, \quad X_{j-1} \le x \le X_j \tag{6.3}$$

Text Box 6.1

Integrating Eq. 6.1 yields the general solution

$$h^2(x) = -\frac{N}{K}(x - X_{j-1})^2 + C_1(x - X_{j-1}) + C_2, \quad X_{j-1} \le x \le X_j$$

where C_1 and C_2 are arbitrary constant. To obtain the particular solution of our problem, we need find C_1 and C_2 based on the boundary conditions at the ends of intervals, at locations: $X_1 = 25$ $X_0 = 25$, $X_2 = 50$, $X_3 = 75$ and $X_4 = L = 100$ m. It follows from the fist condition 6.2 that $C_2 = h_2^2(X_{j-1})$. To find C_1, we have to write the equation for flux at the same location X_{j-1}:

$$2K\left(h(x)\frac{dh(x)}{dx} \right) \Big|_{x=X_{j-1}} = 2N(L - X_{j-1}) = -2\frac{N}{K}(x - X_{j-1})\big|_{x=X_{j-1}} + C_1 = C_1$$

So, $C_1 = 2\ N(L - X_{j-1})$, and the particular solution, Eq. 6.3 follows

The squared thickness of the aquifer $h_{j\ =\ 1,\ \ldots,\ 4}$ observed at locations X_1, X_2, X_3 and X_4 follows from Eq. 6.3:

$$h_j^2 = h_{j-1}^2 + \frac{N}{K_j}(2L - X_{j-1} - X_j)(X_j - X_{j-1}) \tag{6.4}$$

Let the simulation geological model consist of two homogeneous blocks with the boundary between them at location $X = 50$ m. The goal is evaluating two effective hydraulic conductivities, $\hat{K}_1$ and $\hat{K}_2$, for the model blocks based on observations on the thicknesses of the aquifer at locations: $X_1 = 25$, $X_2 = 50$, $X_3 = 75$, and $X_4 = 100$ m selected to simplify calculations. The simulated thickness of the aquifer at those locations can be calculated as

$$\hat{h}_j^2 = \hat{h}_{j-1}^2 + \frac{N}{\hat{K}_i}\left(2X_4 - X_j - X_{j-1}\right)\left(X_j - X_{j-1}\right), \quad i = 1, 2; \quad j = 1, 2, 3, 4 \tag{6.5}$$

(The effective hydraulic conductivity $\hat{K}_1$ substitutes for K_1 and K_2, and $\hat{K}_2$ for K_3 and K_4.) The goodness of fit for the parameters $\hat{K}_1$ and $\hat{K}_2$ is evaluated by criterion

$$s = \sum_{j=1}^{4} p_j \left(\hat{h}_j^2 - h_j^2\right)^2 \tag{6.6}$$

in which the weight p_j assigns the significance of the squared differences between the observed and simulation results at location X_j. Substituting in Eq. 6.5, the given values of $X_0 = 0, X_1 = 25, X_2 = 50, X_3 = 75, X_4 = 100$ m and $N = 0.0001$ m/day yields

$$\begin{aligned}
h_1^2 &= h_0^2 + 0.4375\ g_1 \\
h_2^2 &= h_0^2 + 0.4375\ g_1 + 0.3125\ g_2 \\
h_3^2 &= h_0^2 + 0.4375\ g_1 + 0.3125\ g_2 + 0.1875\ g_3 \\
h_4^2 &= h_0^2 + 0.4375\ g_1 + 0.3125\ g_2 + 0.1875\ g_3 + 0.0625\ g_4
\end{aligned} \tag{6.7}$$

where $g_1 = 1/K_1$, $g_2 = 1/K_2$, $g_3 = 1/K_3$, $g_4 = 1/K_4$ are the actual specific hydraulic resistivities. The same procedure for simulation results, Eq. 6.5, yields

$$\begin{aligned}
\hat{h}_1^2 &= h_0^2 + 0.4375\ \hat{g}_1 \\
\hat{h}_2^2 &= h_0^2 + 0.75\ \hat{g}_1 \\
\hat{h}_3^2 &= h_0^2 + 0.75\ \hat{g}_1 + 0.1875\ \hat{g}_2 \\
\hat{h}_4^2 &= h_0^2 + 0.75\ \hat{g}_1 + 0.25\ \hat{g}_2
\end{aligned} \tag{6.8}$$

where $\hat{g}_1 = 1/\hat{K}_1$ and $\hat{g}_2 = 1/\hat{K}_2$ are the effective specific hydraulic resistivities. The resistivities are introduced to linearize Eqs. 6.3, 6.4, 6.7 and 6.8 and the transforming mechanisms following from them.

Substituting the simulation results (Eq. 6.8) in Criterion 6.6, yields

$$\begin{aligned}
s = {} & p_1\left(h_0^2 + 0.4375\ \hat{g}_1 - h_1^2\right)^2 + p_2\left(h_0^2 + 0.75\ \hat{g}_1 - h_2^2\right)^2 \\
& + p_3\left(h_0^2 + 0.75\ \hat{g}_1 + 0.1875\ \hat{g}_2 - h_3^2\right)^2 + p_4\left(h_0^2 + 0.75\ \hat{g}_1 + 0.25\ \hat{g}_2 - h_4^2\right)^2
\end{aligned} \tag{6.9}$$

Application of the standard procedure of the least squares method to Sum 6.9 leads to the linear system of equations for calculating the effective values $\hat{g}_1$ and $\hat{g}_2$ based on the observed differences $\left(h_i^2 - h_0^2\right),\ (i = 1, 2, 3, 4)$:

$$\begin{aligned}
&\left(0.4375^2\, p_1 + 0.75^2(p_2 + p_3 + p_4)\right)\hat{g}_1 + 0.75(0.1875\, p_3 + 0.25\, p_4)\hat{g}_2 \\
&\quad = 0.4375\, p_1\left(h_1^2 - h_0^2\right) + 0.75\left(p_2\left(h_2^2 - h_0^2\right) + p_3\left(h_3^2 - h_0^2\right) + p_4\left(h_4^2 - h_0^2\right)\right) \\
&0.75(0.1875\, p_3 + 0.25\, p_4)\, \hat{g}_1 + \left(0.1875^2\, p_3 + 0.25^2\, p_4\right)\hat{g}_2 \\
&\quad = 0.1875\, p_3\left(h_3^2 - h_0^2\right) + 0.25\, p_4\left(h_4^2 - h_0^2\right)
\end{aligned} \tag{6.10}$$

The matrix c of System 6.10 is

$$c = \begin{Bmatrix} 0.4375^2\, p_1 + 0.75^2(p_2 + p_3 + p_4) & 0.75(0.1875\, p_3 + 0.25\, p_4) \\ 0.75(0.1875\, p_3 + 0.25\, p_4) & 0.1875^2\, p_3 + 0.25^2\, p_4 \end{Bmatrix} \tag{6.11a}$$

It depends on structure of the object and simulation model, the observation network and the weights, but not on the observations. The right-hand terms (vector $\boldsymbol{b}$) of System 6.10

$$\boldsymbol{b} = \begin{Bmatrix} 0.4375\, p_1\left(h_1^2 - h_0^2\right) + 0.75\left(p_2\left(h_2^2 - h_0^2\right) + p_3\left(h_3^2 - h_0^2\right) + p_4\left(h_4^2 - h_0^2\right)\right) \\ 0.1875\, p_3\left(h_3^2 - h_0^2\right) + 0.25\, p_4\left(h_4^2 - h_0^2\right) \end{Bmatrix} \tag{6.11b}$$

depends on observations.

The effective hydraulic resistivities are solution of System 6.10:

$$\hat{g}_1 = \Delta_1/\Delta, \quad \hat{g}_2 = \Delta_2/\Delta \tag{6.12a}$$

with determinants:

$$\begin{aligned}
\Delta &= c_{11}c_{22} - c_{12}c_{21} \\
\Delta_1 &= b_1 c_{22} - b_2 c_{12} \\
\Delta_2 &= b_2 c_{11} - b_1 c_{21}
\end{aligned} \tag{6.12b}$$

Expressions 6.12a, 6.12b solve the above formulated model identification problem. To find the mechanisms transforming the actual hydraulic resistivities g_1, g_2, g_3 and g_4 into the effective resistivities $\hat{g}_1$ and $\hat{g}_2$, it is necessary to express vector $\boldsymbol{b}$ (Expressions 6.11b) in terms of the resistivities g_1, g_2, g_3 and g_4.

$$\begin{aligned}
\boldsymbol{b}_1 &= 0.4375(0.4375\, p_1 + 0.75\,(p_2 + p_3 + p_4))\, g_1 \\
&\quad + 0.3125 \times 0.75\,(p_2 + p_3 + p_4)\, g_2 \\
&\quad + 0.1875 \times 0.75(p_3 + p_4)\, g_3 + 0.75 \times 0.0625\, p_4\, g_4 \\
\boldsymbol{b}_2 &= 0.4375(0.1875\, p_3 + 0.25\, p_4)\, g_1 \\
&\quad + 0.3125(0.1875\, p_3 + 0.25\, p_4)\, g_2 \\
&\quad + 0.1875(0.1875\, p_3 + 0.25\, p_4)\, g_3 \\
&\quad + 0.25 \times 0.0625\, p_4\, g_4
\end{aligned} \tag{6.13}$$

and then substitute them in Solution (6.12b). To write the result in a more compact way, let us introduce vectors $\boldsymbol{W}_1$ and $\boldsymbol{W}_2$ constituted by the multipliers of the hydraulic resistivities g_1, g_2, g_3 and g_4 in Eq. 6.13:

$$\begin{aligned}\boldsymbol{W}_1 &= \left\{\begin{array}{c} 0.4375(0.4375\,p_1 + 0.75\,(p_2 + p_3 + p_4)) \\ 0.3125 \times 0.75\,(p_2 + p_3 + p_4) \\ 0.1875 \times 0.75(p_3 + p_4) \\ 0.75 \times 0.0625\,p_4 \end{array}\right\} \\ \boldsymbol{W}_2 &= \left\{\begin{array}{c} 0.4375(0.1875\,p_3 + 0.25\,p_4) \\ 0.3125(0.1875\,p_3 + 0.25\,p_4) \\ 0,1875(0.1875\,p_3 + 0.25\,p_4) \\ 0.25 \times 0.0625\,p_4 \end{array}\right\}\end{aligned} \tag{6.14}$$

Then the affecting factors of the pertinent transforming mechanisms can be calculated as

$$\begin{aligned}\{w_{11}, w_{12}, w_{13}, w_{14}\} &= \left\{\frac{W_1 c_{22} - W_2 c_{21}}{c_{11}c_{22} - c_{12}c_{21}}\right\}^T \\ \{w_{21}, w_{22}, w_{23}, w_{24}\} &= \left\{\frac{W_2 c_{11} - W_1 c_{12}}{c_{11}c_{22} - c_{12}c_{21}}\right\}^T\end{aligned} \tag{6.15}$$

where index 'T' means transposition of the yielded vector of the affecting factors as i.e., their representation as row vectors.

The affecting factors do not depend on values of $\{g_{1:4}\}$. This means that the mechanisms presented by them are linear.

6.2 Illustrative Cases

Several cases are presented in this section to get a better feeling for the transforming mechanisms, their properties and sensitivity to each element of the model identification problem formulation.

Cases 6.2.1 and 6.2.2 These cases differ only with respect to distributions of the actual hydraulic conductivity values (Table 6.1). The weighting is uniform (all weights are the same). The values of the effective hydraulic resistivities for the

Table 6.1 Cases 6.2.1 and 6.2.2: distributions of the hydraulic conductivity values

Intervals (m):	0–25	25–50	50–75	75–100
Hydraulic conductivity (m/day)	K_1	K_2	K_3	K_4
Case 6.2.1	1	0.9	0.2	0.1
Case 6.2.2	0.1	0.2	0.9	1

model blocks 1 (interval [0, 50] m) and 2 (interval [50, 100] m) are evaluated, using the same transforming mechanisms, since their affecting factors, calculated by Eq. 6.15, do not depend on the hydraulic conductivity distributions and are the same for both cases:

$$\begin{aligned} \hat{g}_1 &= 0.6861\ g_1 + 0.3139\ g_2 + 0.0072\ g_3 - 0.0072\ g_4 \\ \hat{g}_2 &= -0.3451\ g_1 + 0.3451\ g_2 + 0.8155\ g_3 + 0.1845\ g_4 \end{aligned} \tag{6.16}$$

Note, that Mechanisms 6.16 have the properties obtained in Sect. 5.3 based on theoretical considerations.

The results for Case 6.2.1 are presented in Table 6.2 and Fig. 6.2. They seem to be satisfying. The maximal error in the aquifer thickness is 0.0538 m at $x = 75$ m. The results of Case 6.2.2 are presented in Fig. 6.2 and in Table 6.3. They are not so good, comparing to the result of Case 6.2.1, with the maximal error in the aquifer thickness equal 0.1708 m at $x = 25$ m. The most disappointing is the negative value of the effective hydraulic conductivity $\hat{K}_2$ which is meaningless physically.

The results of Case 6.2.2 are presented in Fig. 6.2 and in Table 6.3. They are not so good, comparing to the result of Case 6.2.1, with the maximal error in the aquifer thickness equal to 0.1708 m at $x = 25$ m. The most disappointing is

Table 6.2 Case 6.2.1: comparison of factual data and simulation results

Effective conductivity (m/day)	$\hat{K}_1$= 1.0011		$\hat{K}_2$= 0.1678	
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	0.4475	0.7947	1.7322	2.3572
Squared simulation aquifer thickness (m^2)	0.4470	0.7592	1.8766	2.2491

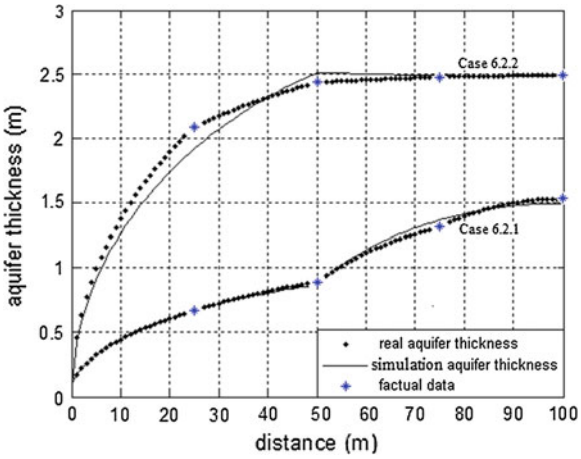

Fig. 6.2 Cases 6.2.1 and 6.2.2: comparison of factual and simulation aquifer thicknesses

Table 6.3 Case 6.2.2: comparison of factual data and simulation results

Effective conductivity (m/day)	$\hat{K}_1 = 0.1186$		$\hat{K}_2 = -1.5751$	
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulation aquifer thickness (m^2)	3.6987	6.3335	6.2144	6.1748

the negative value of the effective hydraulic conductivity $\hat{K}_2$ which is meaningless physically.

The first urge is to disregard Case 6.2.2 as an incorrect formulation of the model identification problem, but what is wrong with the formulation? It does not differ from that of Case 6.2.1. The transforming mechanisms are the same. The effective hydraulic resistivities are unique solutions of linear systems which are stable. What is more important, being physically incorrect, they provide the effective simulation of the water table or the thickness of the aquifer at the observation locations, doing exactly what have been required from them. Sure it would be wrong to apply these hydraulic conductivities to reproducing streamlines, but the streamlines have not been the goal of the optimization.

The negative conductivity has appeared as compensation for a very steep growth of the aquifer thickness near the trench and its very slow growth at the right half of the object, that is, as a consequence of the applied optimization procedure. By the way, the value of effective conductivity $\hat{K}_2$ in Case 6.2.1 is a little greater than the real world hydraulic conductivity K_1. Thus, being correct physically, it is incorrect geologically. In the following cases, this phenomenon demonstrates itself more clearly.

To avoid the use of the negative value of the effective hydraulic conductivity $\hat{K}_2$ and to see how physically based parameters perform in Case 6.2.2, let us try the harmonic averages of the actual hydraulic conductivities as model parameters. (Note, to assign a harmonic average conductivity as a parameter, we have to know the factual values of pertinent hydraulic conductivities. In Cases 6.2.1–6.2.2, the effective hydraulic conductivities were obtained based on the observed thickness of the aquifer by solving System 6.10.)

Case 6.2.3 The effective hydraulic conductivity of the above two blocks is assigned as harmonic means:

$$\hat{K}_1 = \frac{K_1 K_2}{K_1 + K_2} = \frac{0.1 \times 0.2}{0.1 + 0.2} = 0.0667 \text{ m/day}$$

$$\hat{K}_2 = \frac{K_3 K_4}{K_3 + K_4} = \frac{0.9 \times 1}{1.9} = 0.4737 \text{ m/day}$$

Substituting these values of the hydraulic conductivities into Eq. 6.8 yields results presented in Table 6.4 and Fig. 6.3. The advantage of the formulation of the model identification problem in Case 6.2.2 is obvious. (Note also, the above values of the model parameters are not geologically correct.)

Table 6.4 Case 6.2.3: comparison of factual data and simulation results

Effective conductivity (m/day)	$\hat{K}_1 = 0.0667$		$\hat{K}_2 = 0.4737$	
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulation aquifer thickness (m^2)	6.5725	11.2600	11.6558	11.7878

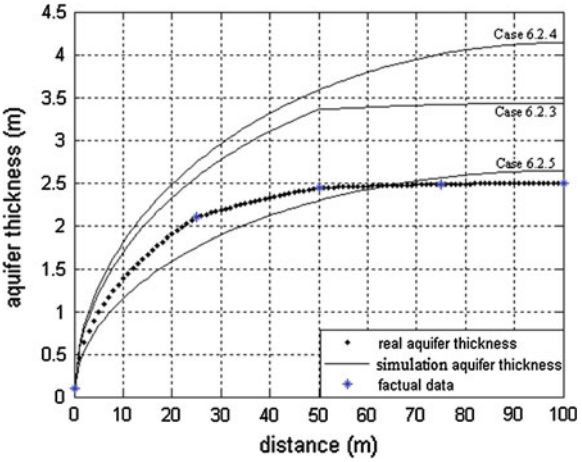

Fig. 6.3 Cases 6.2.3–6.2.5: Comparison of factual and simulation aquifer thickness

Case 6.2.4 Let us try a homogeneous (one block) simulation model with the effective hydraulic conductivity assigned as a harmonic mean of fourth factual values of the hydraulic conductivities:

$$\hat{K} = \frac{1}{\frac{1}{K_1} + \frac{1}{K_2} + \frac{1}{K_3} + \frac{1}{K_4}} = \frac{1}{\frac{1}{0.1} + \frac{1}{0.2} + \frac{1}{0.9} + \frac{1}{1}} = 0.0584 \text{ m/day}$$

The results of Case 6.2.4 are presented in Table 6.5 and in Fig. 6.3. Note, that the above statistics is geologically incorrect again.

Comparison of the results of Cases 6.2.2–6.2.4 demonstrates that the physically incorrect effective parameters perform better, much better, than those assigned from physical and statistical consideration. Besides, the latter are geologically incorrect as well. So, it is up to the modeler to decide what the model parameters are preferable, i.e., simulating results more accurately or yielding less accurate but 'politically correct' results. (Political correctness is mentioned here based on the

Table 6.5 Case 6.2.4: comparison of factual data and simulation results

Effective conductivity (m/day)	$\hat{K} = 0.0584$			
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulation aquifer thickness (m^2)	7.4961	12.8433	16.0517	17.1211

author experience: each time when the efficiency of the physically incorrect parameters was demonstrated, hydrogeologists object to them just because of their physical incorrectness.)

Case 6.2.5 It is interesting also to compare Cases 6.2.3 and 6.2.4 with the homogeneous (one block) model optimized in the sense of Criterion 6.6 with uniform weighting ($p_j = 1$, $j = 1, 2, 3, 4$). The corresponding effective hydraulic resistivity in this case is equal to:

$$\hat{g} = \frac{0.4375\left(h_1^2 - h_0^2\right) + 0.75\left(h_2^2 - h_0^2\right) + 0.9375\left(h_3^2 - h_0^2\right) + \left(h_4^2 - h_0^2\right)}{0.4375^2 + 0.75^2 + 0.9375^2 + 1} \tag{6.17}$$

The corresponding transforming mechanism can be obtained by substitution in the above equation the values of differences $\left(h_j^2 - h_0^2\right)$ from Eq. 6.7:

$$\hat{g} = 0.5193\, g_1 + 0.3190\, g_2 + 0.1380\, g_3 + 0.0237\, g_4 \tag{6.18}$$

The results of Case 6.2.5 are presented in Fig. 6.3 and Table 6.6. Although they are worse than the ones in Case 6.2.2, they are considerably better than those of Cases 6.2.3 and 6.2.4.

Case 6.2.6 Let us try some different formulations of the problem. For example, we can assign the weights increasing with the distance from the trench, say, $p_1 = 0.1$, $p_2 = 0.2$, $p_3 = 0.3$, and $p_4 = 0.4$. Corresponding transforming mechanisms are

$$\begin{aligned} \hat{g}_1 &= 0.6407\, g_1 + 0.3593\, g_2 + 0.0133\, g_3 - 0.0133\, g_4 \\ \hat{g}_2 &= -0.1891\, g_1 + 0.1891\, g_2 + 0.7802\, g_3 + 0.2198\, g_4 \end{aligned} \tag{6.19}$$

The results of Case 6.2.6 are presented in Table 6.7 and in Fig. 6.4. The maximal error in the aquifer thickness is 0.2160 m at $x = 25$ m. Although it is a little greater than the maximal error in Case 6.2.2 (0.1708 m), the accuracy of the results in Case 6.2.6 growth with distance due to the choice of the weights.

Table 6.6 Case 6.2.5: comparison of factual data and simulation results

Effective hydraulic conductivity (m/day)	$\hat{K} = 0.1436$			
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulation aquifer thickness (m^2)	3.0572	5.2338	6.5397	6.9750

Table 6.7 Case 6.2.6: comparison of factual data and simulation results

Effective hydraulic conductivity (m/day)	$\hat{K}_1 = 0.1219$		$\hat{K}_2 = 7.0757$	
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulation aquifer thickness (m^2)	3.5997	6.1637	6.1902	6.1990

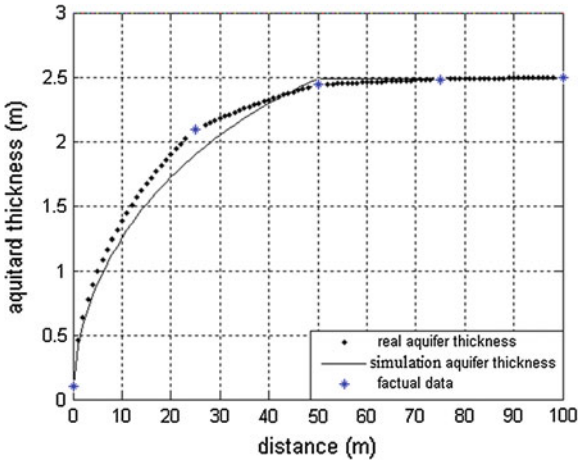

Fig. 6.4 Case 6.2.6: comparison of factual and simulation aquifer thickness

Moreover, the effective conductivity $\hat{K}_2$ is physically correct, positive. However, it is incorrect geologically exceeding the actual hydraulic conductivity K_3 and K_4 considerably. This can make the model as erroneous as the physically incorrect effective value $\hat{K}_2$ in Case 6.2.2 and in some different formulations of the simulation problem.

Case 6.2.7 Let us change the observation network. We come back to the uniform weighting, but move the observation from location $x = 25$ m to $x = 10$ m. This leads to changing the above system composed by the geological object, simulation model, and observation network. Consequently, this leads to different system of equations for finding the effective conductivities and the transforming mechanisms. The effective hydraulic resistivities $\hat{g}_1$ and $\hat{g}_2$ become the solution to the system:

$$\begin{aligned}
&\left(0.19^2 p_1 + 0.75^2(p_2 + p_3 + p_4)\right)\hat{g}_1 + 0.75(0.1875 p_3 + 0.25 p_4)\hat{g}_2 \\
&\quad = 0.19 p_1\left(h_1^2 - h_0^2\right) + 0.75\left(p_2\left(h_2^2 - h_0^2\right) + p_3\left(h_3^2 - h_0^2\right) + p_4\left(h_4^2 - h_0^2\right)\right) \\
&0.75\left(0.1875\, p_3 + 0.25\, p_4\right)\hat{g}_1 + \left(0.1875^{\,2} p_3 + 0.25^{\,2} p_4\right)\hat{g}_2 \\
&\quad = 0.1875\, p_3\left(h_3^2 - h_0^2\right) + 0.25\, p_4\left(h_4^2 - h_0^2\right)
\end{aligned} \tag{6.20}$$

The corresponding transforming mechanisms are

$$\begin{aligned}
\hat{g}_1 &= 0.6076\, g_1 + 0.3924\, g_2 + 0.0091\, g_3 - 0.0091\, g_4 \\
\hat{g}_2 &= -0.0814\, g_1 + 0.0814\, g_2 + 0.8096\, g_3 + 0.1904\, g_4
\end{aligned} \tag{6.21}$$

The results of Case 6.2.7 are presented in Table 6.8 and in Fig. 6.5. The maximal error in the aquifer thickness is 0.1968 m at $x = 25$ m.

Table 6.8 Case 6.2.7: comparison of factual data and simulation results

Effective hydraulic conductivity (m/day)	$\hat{K}_1 = 0.1244$		$\hat{K}_2 = 1.4642$	
Monitoring location (m)	10	50	75	100
Squared factual aquifer thickness (m^2)	1.9100	5.9475	6.1558	6.2183
Squared simulation aquifer thickness (m^2)	1.5373	6.0389	6.1669	6.2096

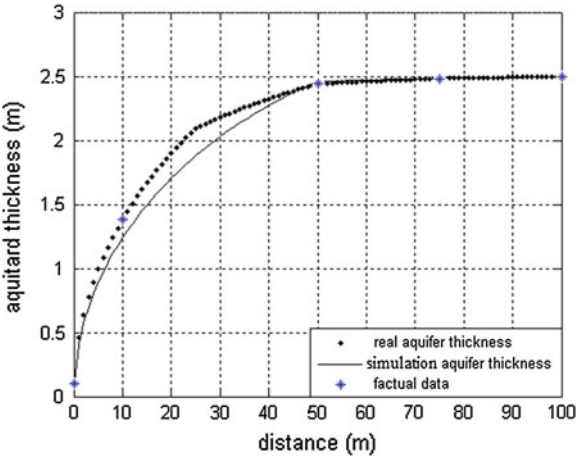

Fig. 6.5 Case 6.2.7: comparison of factual and simulation aquifer thickness

It is worth noting that the model identification in Case 6.2.7 is also geologically incorrect: the effective hydraulic $\hat{K}_2$ exceeds the factual values of the hydraulic conductivity.

Case 6.2.8 Let us consider one more alternative to the model identification problem presented in Case 6.2.2. This time we change the model itself: the first block of the new model coincides with the first geological body (interval [0, 25] m). The second block (interval (25, 100] m) consists of three geological bodies. The observation network and weights are the same as in Case 6.2.2. The system of equations for finding effective values $\hat{g}_1$ and $\hat{g}_2$ is

$$\begin{aligned}
&0.4375(p_1 + p_2 + p_3 + p_4)\hat{g}_1 + (0.3125\, p_2 + 0.5p_3 + 0.5625\, p_4)\hat{g}_2 \\
&\quad = p_1\left(h_1^2 - h_0^2\right) + p_2\left(h_2^2 - h_0^2\right) + p_3\left(h_3^2 - h_0^2\right) + p_4\left(h_4^2 - h_0^2\right) \\
&0.4375(0.3125\, p_2 + 0.5p_3 + 0.5625\, p_4)\hat{g}_1 + \left(0.3125^2\, p_2 + 0.5^2\, p_3 + 0.5625^2\, p_4\right)\hat{g}_2 \\
&\quad = 0.3125\, p_2\left(h_2^2 - h_0^2\right) + 0.p_3\left(h_3^2 - h_0^2\right) + 0.5625\, p_4\left(h_4^2 - h_0^2\right)
\end{aligned} \tag{6.22}$$

The transforming mechanisms in this case are:

$$\begin{aligned}
\hat{g}_1 &= 1 \times g_1 + 0.0948\, g_2 - 0.0743\, g_3 - 0.0205\, g_4 \\
\hat{g}_2 &= 0 \times g_1 + 0.5612\, g_2 + 0.3673\, g_3 + 0.0715\, g_4
\end{aligned} \tag{6.23}$$

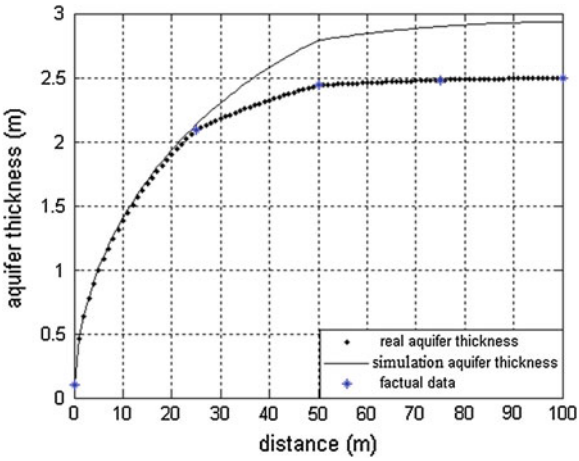

Fig. 6.6 Case 6.2.8: comparison of factual and simulation aquifer thickness

Table 6.9 Case 6.2.8: comparison of factual data and simulation results

Effective hydraulic conductivity (m/day)	$\hat{K}_1 = 0.0964$		$\hat{K}_2 = 0.3043$	
Monitoring location (m)	25	50	75	100
Squared factual aquifer thickness (m^2)	4.3850	5.9475	6.1558	6.2183
Squared simulation aquifer thickness (m^2)	4.5472	7.7881	8.4041	8.6095

The results of Case 6.2.8 are presented in Fig. 6.6 and Table 6.9. The maximal error in the aquifer thickness is 0.4405 m at $x = 100$ m. In general, the results are considerably worse than those in Cases 6.2. The effective parameters are incorrect geologically. However, the accuracy of reproducing the aquifer thickness in interval [0, 25] m is impressive. Maybe, it is worth to contemplate application of different models to different parts of geological objects.

6.3 Discussion on Illustrative Cases

Table 6.10 summarizes the results of Sect. 6.2. The cases demonstrate clearly the problem dependence of model identification and support statement that "it is not possible to define a consistent effective parameter value to reproduce the response of a spatially variable pattern of parameter values" (Beven 1989). We see that the effective parameters of predictive models and the transforming mechanisms depend on geological conditions (Cases 6.2.1 and 6.2.2), and literally on each element of simulation problem formulation (Cases 6.2.2 and 6.2.5–6.2.8). All transforming mechanisms have Properties 1–3, and they are not statistics, besides that presented by Eq. 6.18.

Table 6.10 Transforming mechanisms and effective hydraulic resistivities $\hat{G}$ (day/m) and conductivities $\hat{K} = 1/\hat{G}$ (m/day)

Case	Equation #	Transforming mechanism	Effective parameters $\hat{g}$, $\hat{K} = 1/\hat{g}$
6.2.1	1	$\hat{g}_1 = 0.6861\ g_1 + 0.3139\ g_2 + 0.0072\ g_3 - 0.0072\ g_4$	$\hat{g}_1 = 0.9989,\ \hat{K}_1 = 1.0011$
	2	$\hat{g}_2 = -0.3451\ g_1 + 0.3451\ g_2 + 0.8157\ g_3 + 0.1843\ g_4$	$\hat{g}_2 = 5.9595,\ \hat{K}_2 = 0.1678$
6.2.2	3	$\hat{g}_3 = 0.6861\ g_1 + 0.3139\ g_2 + 0.0072\ g_3 - 0.0072\ g_4$	$\hat{g}_3 = 8.4311,\ \hat{K}_3 = 0.1186$
	4	$\hat{g}_4 = -0.3451\ g_1 + 0.3451\ g_2 + 0.8157\ g_3 + 0.1843\ g_4$	$\hat{g}_4 = -0.6351,\ \hat{K}_4 = -1.5746$
6.2.5	5	$\hat{g}_5 = 0.5193\ g_1 + 0.3190\ g_2 + 0.1380\ g_3 + 0.0237\ g_4$	$\hat{g}_5 = 7.2516,\ \hat{K}_5 = 0.1379$
6.2.6	6	$\hat{g}_6 = 0.6407\ g_1 + 0.3593\ g_2 + 0.0133\ g_3 - 0.0133\ g_4$	$\hat{g}_6 = 8.2034,\ \hat{K}_6 = 0.1219$
	7	$\hat{g}_7 = -0.1891\ g_1 + 0.1891\ g_2 + 0.7802\ g_3 + 0.2198\ g_4$	$\hat{g}_7 = 0.1413,\ \hat{K}_7 = 7.0757$
6.2.7	8	$\hat{g}_8 = 0.6076\ g_1 + 0.3924\ g_2 + 0.0091\ g_3 - 0.0091\ g_4$	$\hat{g}_8 = 8.0386,\ \hat{K}_8 = 0.1244$
	9	$\hat{g}_9 = -0.0814\ g_1 + 0.0814\ g_2 + 0.8096\ g_3 + 0.1904\ g_4$	$\hat{g}_9 = 0.6830,\ \hat{K}_9 = 1.4642$
6.2.8	10	$\hat{g}_{10} = 1\ \times\ g_1 + 0.0948\ g_2 - 0.0743\ g_3 - 0.0205\ g_4$	$\hat{g}_{10} = 10.3734,\ \hat{K}_{10} = 0.0964$
	11	$\hat{g}_{11} = 0\ \times\ g_1 + 0.5612\ g_2 + 0.3673\ g_3 + 0.0715\ g_4$	$\hat{g}_{11} = 3.2862,\ \hat{K}_{11} = 0.3043$

The problems in Sect. 6.2 are linear with respect to squared thickness of the aquifer. Therefore they do not support the most popular explanation of the problem-dependence phenomenon by non-linearity of simulation processes. Being results of optimization, the effective parameters are not physical or geological entities. They are characteristics of the system made up not only by geological objects but as well all elements of the model identification problem formulations. That is why the effective parameters can be incorrect physically and geologically but still remain effective in pertinent optimizations. However, they can become misleading, if predictive simulations deal with the systems different from those in which the parameters are obtained. Case 6.2.2 is revealing in this sense. The effective hydraulic conductivities $\hat{K}_1 = 0.1186$ and $\hat{K}_2 = -1.5751$ m/day satisfactory reproducing the aquifer thickness are misleading in evaluations of streamlines which are not a subject of optimization in the calibration.

On earlier stages of investigation, exact formulations of simulation problems may not be known yet. Then the goal of the model identification is finding geologically correct parameters, i.e., the model characteristics must be within the range of factual properties of the geological object of interest. The transforming mechanism like in Case 6.2.5, being averaging of the statistical nature, can serve to such end. But to be sure that the effective parameter values are indeed averaging of the statistical nature, the transforming mechanisms must be presented explicitly.

Contrary to seeing the problem-dependence as an obstacle or annoying factor, it is more profitable to consider it as a tool for investigation of geological objects. Different formulations of the model identification problems and corresponding transforming mechanisms carry information about the structures and properties of geological objects. They even can be applied to formulating and solving inverse problems. Geophysics is an example of such use of the phenomenon of problem-dependency. The notion of the apparent electrical resistivity corresponds to the effective parameters as they are defined in the hydrogeological model identification herein. Namely, the apparent specific electrical resistivity provides the exact difference of electrical potentials between the receiving electrodes for a given configuration of the current electrodes. Its value is calculated based on assumption that the geological object is homogeneous with respect to the specific electrical resistivity. If the actual object is not homogeneous, changing the configuration of the current electrodes, which is equivalent to changing the boundary conditions (or locations of sources and sinks), leads to change of the apparent resistivity. The pattern of the changing is used for qualitative or quantitative interpretation of the object structure.

Let us consider the following system of equations:

$$\begin{aligned} 0.6861\ g_1 + 0.3139\ g_2 + 0.0072\ g_3 - 0.0072\ g_4 &= 8.4311 \\ -0.3451\ g_1 + 0.3451\ g_2 + 0.8157\ g_3 + 0.1843\ g_4 &= -0.6351 \\ 0.6076\ g_1 + 0.3924\ g_2 + 0.0091\ g_3 - 0.0091 g_4 &= 8.0386 \\ -0.0814\ g_1 + 0.0814\ g_2 + 0.8096\ g_3 + 0.1904\ g_4 &= 0.6930 \end{aligned} \tag{6.24}$$

System 6.3.1 is composed from Eqs. 3, 4, 8, 9 (Table 6.10). The actual hydraulic resistivities $g_{1:4}$ are assumed to be unknown. Corresponding effective hydraulic resistivities, the right-hand terms are found from observations and as such they are known. Solving System 6.3.1 for the unknown actual resistivities and recalculating them in the actual hydraulic conductivities yield:

$$K_1 = 0{,}1; \quad K_2 = 0{,}2; \quad K_3 = 0{,}9; \quad K_4 = 1{,}0 \text{ м/сутки} \tag{6.25}$$

This is the exact actual properties of the considered object.

Inverse problems are incorrect inherently. The source of incorrectness is errors in the coefficients making up the matrix of System 6.24 and in the right-hand vector. Solutions of the systems like System 6.3 depend strongly on the accuracy of the initial data and rounding errors (see Eq. 4.20). The above success is due to the fact that the made up artificial situation permits calculating values of the affecting factors and effective parameters with accuracy of fourteen digits. If solving the inverse problem with the data presented in Table 6.10, that is, with four significant digits, the result becomes

$$K_1 = 0{,}1; \quad K_2 = 0{,}1997; \quad K_3 = 0{,}9109, \quad K_4 = 0{,}9622 \quad \text{м/сутки} \tag{6.26}$$

which is appropriate still. If the system for finding the actual hydraulic resistivity is made up by Eqs. 3, 4 and 6, 7 from Table 6.10 and the pertinent values rounded up to three digits to the right from the decimal point the obtained solution is not so good:

$$K_1 = 0.0997,\ K_2 = 0.2030,\ K_3 = 0.8137,\ K_4 = 1.4905 \text{ m/day} \tag{6.27}$$

though it can be acceptable, considering the usual accuracy of hydrogeological information. Some systems made up from other combinations of four equations represented in Table 6.10 may yield much worse results.

In day-to-day practice to have four correct significant digits is an unavailable luxury. More practical approach to solving our inverse problem is to use excessive systems of equations and solve them by the least squares method. For example, the affecting factors in Eqs. 3–11 from Table 6.10 can be considered as independent variables and the unknown the actual values g_1, g_2, g_3, g_4 as coefficients of the linear regression

$$\hat{g}_j = g_1 w_{j1} + g_2 w_{j2} + g_3 w_{j3} + g_4 w_{j4} \tag{6.28}$$

(Due to the Properties 1–3 the affecting factors are not independent. This does not preclude considering them as such. However, the dependence of the affecting factors can simplify solving inverse problems.)

Applying the least squares method to minimize sum

$$s = \sum_{j=3}^{11} \left(g_1 w_{j1} + g_2 w_{j2} + g_3 w_{j3} + g_4 w_{j4} - \hat{g}_j \right)^2 \tag{6.29}$$

yields the system of four equations for evaluating regression coefficients g_1, g_2, g_3, g_4. Solution of that system expressed in terms of the hydraulic conductivities is

$$K_1 = 0.0995,\ K_2 = 0.1981,\ K_3 = 0.8627,\ K_4 = 1.1594 \text{ m/day} \qquad (6.30)$$

This approach to solving inverse problems, using the transforming mechanisms is considered in more details in Chap. 9.

Konikow and Bredehoeft (1992) claim that a site specific validation "per se, is a futile objective." In my opinion, they are wrong. We just should stop looking at calibration as at the procedure of searching for the effective parameters of a given model which provide the best fit of the available observations and start seeing it as a procedure for systematic study of the hydrogeological objects. The transforming mechanisms may become a tool for this kind of investigations, though I believe that other tools can be found also.

6.4 Borden Landfill

I think that Frind and Hokkanen (1987) assigned their recharge rate pattern and the steady-state water table for the part of the Borden site located down-gradient of the landfill ($x > 300$ m) in Sect. 4.4, taking in consideration the observed streamline which coincides with the upper boundary of the contaminant plume. Then they scaled the recharge pattern and the hydraulic conductivities to satisfy the approximately known arrival time. The goal of this section is obtaining the mechanism transforming the recharge rates N_3, N_4, and N_5 into one effective recharge rate $\hat{N}$ of the homogeneous simulation model for $x > 300$ m (Fig. 6.7).

The effective recharge rate $\hat{N}$ should provide the effective, as if, steady-state water table. (Note that if the structure of the model of Frind and Hokkanen (1987) in Sect. 4.4 were an exact replica of the Borden site, then effective recharge rates were equal to the actual recharges, i.e. $\hat{N}_3 = N_3$, $\hat{N}_4 = N_4$ and $\hat{N}_5 = N_5$, and as shown in Sect. 5.3, the corresponding transforming mechanisms with affecting factors $w_{1,1} = w_{2,2} = w_{3,3} = 1$, $w_{1,2} = w_{1,3} = w_{2,1} = w_{2,3} = w_{3,1} = w_{3,2} = 0$ become trivial.)

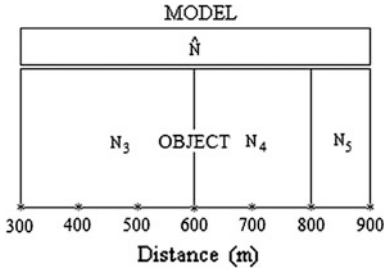

Fig. 6.7 Borden site: model homogeneous with respect to recharge rate

The transforming mechanisms for the homogeneous model can be presented as

$$\hat{N} = w_1 N_3 + w_2 N_4 + w_3 N_5 \tag{6.31}$$

where the affecting factors w_1, w_2 and w_3 are summing to one. According to Eq. 4.35, the actual water table $H(x)$ for $x > x_{st}$ is described by equation

$$H(x) = \frac{Q(x)}{Q_S}(H_S(x) - Y(x)) + Y(x) \tag{6.32}$$

where $H_S(x)$ is the streamline S elevation, $Y(x)$ is the aquifer base elevation, $Q(x)$ is the total flux, and $Q_S = Q(x_{st})$, where x_{st} is the coordinate of the point of the streamline S on the water table.

The effective water table $\hat{H}(x)$ is described by equation

$$\hat{H}(x) = \frac{\hat{Q}(x)}{Q_S}(H_S(x) - Y(x)) + Y(x) \tag{6.33}$$

where $\hat{Q}(x)$ is the effective total flux at $x > x_{st}$. The effective value of the homogeneous recharge rate $\hat{N}$ minimize the sum

$$s = \sum_{i=1}^{n} \left(\hat{H}(x_i) - H(x_i)\right)^2 \tag{6.34}$$

where x_i is the locations where values $H(x)$ $Y(x)$ and $H_S(x)$ are observed. However observations on $H(x)$ are not necessary and even may not exist in this case. Indeed, substituting Eqs. 6.32–6.33 in Criterion 6.34 yields

$$s = \frac{1}{Q_S^2} \sum_{i=1}^{n} \left(\left(\hat{Q}(x_i) - Q_i(x_i)\right)(H_S(x_i) - Y(x_i))\right)^2 \tag{6.35}$$

So the problem is reduced to evaluating the effective recharge rate based on an observed streamline. According to the least squares method the effective recharge rate $\hat{N}$ is the solution of equation

$$\sum_{i=1}^{n} \left(\left(\hat{Q}(x_i) - Q(x_i)\right)(H_S(x_i) - Y(x_i))\right) \frac{d\hat{Q}(x_i)}{d\hat{N}} = 0 \tag{6.36}$$

Substituting the data from Table 6.11 in Eq. 6.36 and solving it for $\hat{N}$ yield Eq. 6.31 with $w_1 = 0.8005$, $w_2 = 0.1727$, $w_3 = 0.0269$ summing to 1.0001. (The error 0.0001 is due to rounding. Adding one more digit, i.e. putting $w_1 = 0.80045$, $w_2 = 0.17267$, $w_3 = 0.02688$ makes summing equal to one.) So finally, the transforming mechanisms converting the recharge rates N_3, N_4, and N_5 into the effective recharge rate $\hat{N}$ is

$$\hat{N} = 0,8005\, N_3 + 0,1727\, N_4 + 0,0269\, N_5 \tag{6.37}$$

Table 6.11 Data for evaluating transforming mechanism for effective recharge rate

#	x	H_S	Y	$u = H_S - Y$	$\hat{Q}$	Q
0	300	222.31	204.31	17.99	Q_S	Q_S
1	400	219.25	206.17	13.08	$Q_S + 100\hat{N}$	$Q_S + 100\ N_3$
2	500	218.26	209.55	8.71	$Q_S + 200\hat{N}$	$Q_S + 200\ N_3$
3	600	217.46	210.85	6.61	$Q_S + 300\hat{N}$	$Q_S + 300\ N_3$
4	700	216.07	211.33	4.74	$Q_S + 400\hat{N}$	$Q_S + 300\ N_3 + 100\ N_4$
5	800	215.47	211.86	3.61	$Q_S + 500\hat{N}$	$Q_S + 300\ N_3 + 200\ N_4$
6	900	215.67	212.79	2.88	$Q_S + 600\hat{N}$	$Q_S + 300\ N_3 + 200\ N_4 + 100\ N_5$

Substituting into Eq. 6.37 the recharge pattern $N_{1:5} = [5.85, 28.41, 10.20, 23.00, 8.36]$ cm/year (Table 4.4) which satisfies the streamline shape and the travel times to $x = 900$ m and $x = 950$ m (about 39.1 and 40.2 years) yields the effective recharge

$$\hat{N} = 0.8005 \times 10.2 + 0.1727 \times 23 + 0.0269 \times 8.36 = 12.36 \text{ cm/year} \quad (6.38)$$

To obtain Mechanism 6.37 we do not need the observation on the water table, and the total flux Q_S at $x = 300$ m. Taking in consideration the seasonal variability of the water table which is expected to be greater than the variability of the streamline elevations, the water table obtained with the use of the effective recharge $\hat{N}$ seems to be a better first approximation. However, the above result $\hat{N} = 12.36$ cm/year can be checked by straightforward calculation of the effective recharge applying the observed water table. To this end it is necessary to minimize criterion

$$s = \sum_{i=1}^{6} \left(\frac{\hat{Q}_i}{Q_S} ((H_S(x_i) - Y(x_i)) - (H(x_i) - Y_i)) \right)^2 \quad (6.39)$$

with $H(x)$ corresponding to the above mention recharge pattern from Table 4.4 ($N_{1:5} = [5.85, 28.41, 10.20, 23.00, 8.36]$ cm/year). The data for calculation are presented in Table 6.12 Note also, the effective recharge rate of the model which is

Table 6.12 Data for evaluating the transforming mechanism for effective recharge rate $\hat{N}$ $\left(rN = \hat{N}/Q_S\right)$

#	x	H	$v = H - Y$	Y	H_S	$u = H_S - Y$	$\hat{Q}/Q_S$
0	300	222.31	17.99	204.31	222.31	17.99	1
1	400	222.23	16.06	206.17	219.25	13.08	$1 + 100rN$
2	500	222.11	12.56	209.55	218.26	8.71	$1 + 200rN$
3	600	221.95	11.09	210.85	217.46	6.61	$1 + 300rN$
4	700	221.72	10.39	211.33	216.07	4.74	$1 + 400rN$
5	800	221.42	9.56	211.86	215.47	3.61	$1 + 500rN$
6	900	221.04	8.24	212.79	215.67	2.88	$1 + 600rN$

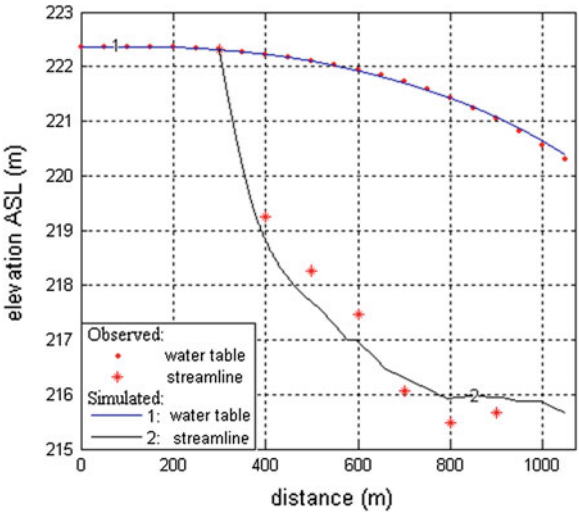

Fig. 6.8 Reproduction of observations by the homogeneous model

homogeneous with respect to recharge for $x > 300$ m must minimize the difference between the observed water table and the simulated one.

The minimum value of the Criterion 6.39 depends on ratio $\hat{Q}_i/Q_S$. Thus the goal is to find the optimal value of this ratio, denoted here as rN. The standard least squares technique leads to equation

$$\begin{aligned} 100\left(u_1^2 + 4u_2^2 + 9u_3^2 + 16u_4^2 + 25u_5^2 + 36u_6^2\right) rN \\ = u_1(v_1 - u_1) + 2u_2(v_2 - u_2) \\ +3u_3(v_3 - u_3) + 4u_4(v_4 - u_4) + 5u_5(v_5 - u_5) + 6u_6(v_6 - u_6) \end{aligned} \tag{6.40}$$

According to Eq. 6.40 $rN = 0.0027$. Calculated based on recharge rates $N_{12} = [5.85,\ 28.41]$ cm/year the total flux Q_S at $x = x_{st} = 300$ m is equal 0.1253 m^2/day. Thus the effective recharge rate is

$$\hat{N} = rN \times Q_s \times 100 \times 365 = 12.40 \text{ cm/year} \tag{6.41}$$

The results obtained by Eqs. 6.38 and 6.41 consistent though based on slightly different data. Thus, the transforming mechanism presented by Eq. 6.38, as expected, provides effective parameter $\hat{N}$ for the discussed simulation model. The magnitude of the maximal error in reproducing the water table is less than 9.1 cm. However, the magnitude of the maximal error in evaluation the streamline starting at $x = 300$ m is too large, about 0.56 m (Fig. 6.8), since the streamline was not the goal of reproduction. Nevertheless the travel time to $x = 900$ m and $x = 950$ m are equal approximately to 38.5 and 39.7 years is close to those found in Sect. 4.4 (39.1 and 40.2 years).

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Chapter 7
Examples of Nonlinear Transforming Mechanisms

Linear transforming mechanisms are rare in practical applications. Even the mechanisms presented in Sect. 6.2 were obtained by linearization of non-linear mechanisms. Mathematical descriptions of the non-linear mechanisms and their inferences and applications are considerably more complicated. However, it is possible to find simple examples for illustrations.

7.1 Simulation of Transient Filtration in Two-Body Object by Homogeneous Model: Problem Formulation

As shown in Sect. 4.3, a homogeneous model with constant hydraulic transmissivity and storativity cannot successfully represent the development of hydraulic heads in a confined aquifer consisting of two geological bodies with the hydraulic transmissivities T_1 and T_2 (Fig. 7.1). However, the situation is different, if we use the effective hydraulic transmissivity changing in time.

Let the aquifer have uniform distribution of the hydraulic heads in the initial state: $h(x, 0) = H_0$. At instant $t = 0$, the hydraulic head at $x = 2L$ jumps to $h(2L, 0) = H_{2L}$. At $x = 0$ the hydraulic head remains unchanged: $h(0, t) = H_0$. The instant jump of the hydraulic head at $x = 2L$ initiates process of changing the aquifer hydraulic heads. The goal is effective simulation of the hydraulic head at location $x = L$, using a homogeneous, one-block, model.

Filtration within two geological bodies, that is, within intervals $[0, L]$ and $[L, 2L]$ is described by two partial differential equations

$$\frac{\partial h_j(x,t)}{\partial t} = A_j \frac{\partial^2 h_j(x,t)}{\partial x^2} \quad j = 1, 2 \tag{7.1}$$

where x and t are the distance and the time, $h_j(x, t)$ is the hydraulic head in intervals $[0, L]$ ($j = 1$) or $[L, 2L]$ ($j = 2$), $A_j = T_j/S$ is the hydraulic diffusivity of body j, T_j is its transmissivity and S is the storativity which, for the sake of

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*, Springer Hydrogeology, DOI: 10.1007/978-3-319-03569-7_7,

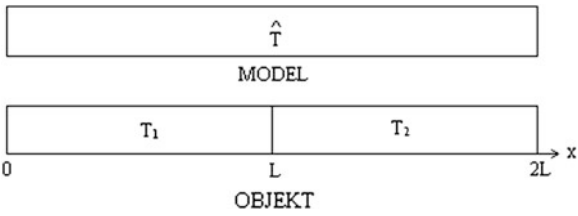

Fig. 7.1 Modeling a two-body object by a homogeneous model

simplicity, is assigned equal to 0.1 for both bodies. The initial and boundary conditions are the following:

$$h_j(x,\,0) = H_0, \quad j = 1, 2; \quad 0 \le x \le 2L \tag{7.2}$$

$$h_1(0,\,t) = H_0 \quad \text{and} \quad h_2(2L,\,t) = H_{2L} \tag{7.3}$$

The inner boundary conditions on continuity of the hydraulic head and the flux exist at the boundary between the geological bodies at $x = L$

$$\begin{aligned} &h_1(L,t) = h_2(x,t) = h(L,t) \\ &T_1 h_1(L,t) \left(\frac{\partial\, h_1(x,t)}{\partial\, x}\right)\Bigg|_{x\to L} = T_2 h_2(L,t) \left(\frac{\partial\, h_2(x,t)}{\partial\, x}\right)\Bigg|_{L\leftarrow x} \end{aligned} \tag{7.4}$$

The real world made up in the above problem formulation is to be simulated by a homogeneous model. The corresponding simulation process is described by equation

$$\frac{\partial\, \hat{h}(x,t)}{\partial\, t} = \hat{A}\, \frac{\partial^2 \hat{h}(x,t)}{\partial\, x^2} \tag{7.5}$$

where $\hat{h}(x,t)$ is the effective hydraulic head at location x and at time instant t, $\hat{A} = \hat{T}/S$ and $\hat{T}$ is the effective hydraulic transmissivity. Model storativity S is assigned equal to 0.1.

The simulation must reproduce effectively the next hydraulic head, $\hat{h}(L, t_i) = \hat{h}_i$, based on the observed previous head $h(L, t_{i-1}) = h_{i-1}$. For simplicity, time increment $\Delta t = t_i - t_{i-1}$ is constant. The simulations are to be conducted by the explicit finite differences. The model must be effective in time interval $[t_{k,}\ t_m]$ in the sense of the least squares, that is, the simulated hydraulic heads must minimize sum

$$s_{k,m} = \sum_{i=k}^{m} \left(\hat{h}_i - h_i\right)^2 \tag{7.6}$$

To this end the effective hydraulic transmissivity, $\hat{T}_{k,m}$, the only parameter governing the simulation, must be found.

7.2 Explicit Numerical Simulation

There exists an analytical solution for the hydraulic heads in the above formulated problem. However, to simplify obtaining the pertinent transforming mechanism, the explicit finite difference method with the stencil presented in Fig. 7.2 is applied to simulate both, the real world and the homogeneous model. (To simplify calculations, the boundary conditions are assigned as $H_0 = h(0,t) = 0$ и $H_{2L} = h(2L,t) = 1$ m).

The equation for evaluating the real world hydraulic head based on the immediately preceding observed hydraulic head is

$$h_i \approx h_{i-1} + \frac{\Delta t}{S L^2}\left(\left(1 - h_{i-1}\right) T_2 - h_{i-1} T_1\right) \tag{7.7}$$

where $h_i = h\,(L,\, t_i)$, $\Delta t = t_i, - t_{i-1} = const$. The hydraulic heads simulated on the homogeneous aquifer model with the effective hydraulic conductivity $\hat{T}_{k,m}$ can be obtained from Eq. 7.7 by putting $T_1 = T_2 = \hat{T}_{k,m}$

$$\hat{h}_i \approx h_{i-1} + \frac{\Delta t}{SL^2}(1 - 2h_{i-1})\hat{T}_{k,m} \tag{7.8}$$

Then Criterion 7.6 can be written as

$$s = \frac{\Delta t}{SL^2} \sum_{i=k+1}^{m} \left((1 - 2h_{i-1})\hat{T}_{k,m} - ((1 - h_{i-1})T_2 - h_{i-1}T_1)\right)^2 \tag{7.9}$$

Applying to Eq. 7.9 the standard least squares technique, that is, differentiating it by $\hat{T}_{k,m}$ and equalizing the derivative to zero, yields

$$\hat{T}_{k,m} = -\frac{\sum_{i=k}^{m} h_{i-1}(1 - 2h_{i-1})}{\sum_{i=k}^{m} (1 - 2h_{i-1})^2} T_1 + \frac{\sum_{i=k}^{m} (1 - h_{i-1})(1 - 2h_{i-1})}{\sum_{i=k}^{m} (1 - 2h_{i-1})^2} T_2, \quad k > 0 \tag{7.10}$$

Equation 7.10 can be rewritten in terms of the affecting factors

$$\hat{T}_{k,m} = w_{1,[k,m]} T_1 + w_{2,[k,m]} T_2 \tag{7.11}$$

where the affecting factors $w_{1,[k,m]}$ and $w_{2,[k,m]}$ are

$$w_{1,[k,m]} = -\frac{\sum_{i=k}^{m} h_{i-1}(1 - 2h_{i-1})}{\sum_{i=k}^{m} (1 - 2h_{i-1})^2}, \quad w_{2,[k,m]} = \frac{\sum_{i=k}^{m} (1 - h_{i-1})(1 - 2h_{i-1})}{\sum_{i=k}^{m} (1 - 2h_{i-1})^2}, \quad k > 0 \tag{7.12}$$

It is easy to check that the above affecting factors hold Property 1 (Sect. 5.3, Eq. 5.5), summing to one. However, they can have different signs. If in interval $[t_k, t_m]$ all h_{i-1} are less than 0.5 m, $w_{1,[k,m]}$ is negative and $w_{2,[k,m]}$ is positive. If in interval $[t_k,\, t_m]$ all h_{i-1} are greater than 0.5 m, $w_{1,[k,m]}$ is positive and $w_{2,[k,m]}$ is negative. Therefore, the effective hydraulic transmissivity $\hat{T}_{k,m}$ are not statistics of the

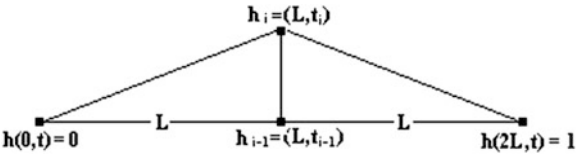

Fig. 7.2 Four point stencil for numerical modeling of the hydraulic heads

hydraulic conductivities T_1 and T_2, though the affecting factors in Eq. 7.11 sum to one.

It is somehow more cumbersome to see non-linearity of Mechanism 7.11. But in the case of the effective parameter $\hat{T}_{1,2}$ this is fairly obvious. It follows from the initial Condition 7.2 and Eq. 7.7 that

$$h_0 = 0 \quad \text{and} \quad h_1 \approx \frac{\Delta t}{SL^2} T_2$$

Substituting the above values in Eq. 7.12 yields

$$w_{1,[1,2]} = -\frac{\left(1 - 2\frac{\Delta t}{SL^2}T_2\right)\frac{\Delta t}{SL^2}T_2}{1 + \left(1 - 2\frac{\Delta t}{SL^2}T_2\right)^2}, \quad w_{2,[1,2]} = \frac{1 + \left(1 - \frac{\Delta t}{SL^2}T_2\right)\left(1 - 2\frac{\Delta t}{SL^2}T_2\right)}{1 + \left(1 - 2\frac{\Delta t}{SL^2}T_2\right)^2}$$

Thus, the affecting factors $w_{1,[1,2]}$ and $w_{2,[1,2]}$ depend on T_2, demonstrating non-linearity of the corresponding transforming mechanism. Note that the above factors do not depend on transmissivity T_1. This fact is useful when the transforming mechanisms are applied for formulations and solving inverse hydrogeological problems Chap. 9. Note also that transmissivity T_1 appears in the transforming mechanisms $\hat{T}_{2,3}$, $\hat{T}_{1,3}$ and all others with $m \geq 3$.

Let us simplify the problem even more, requesting that the effective transmissivity $\hat{T}_{i-1,i}$ should provide exact reproduction of the hydraulic head $h_i = h(L, t_i)$, at instant t_i based on the observed hydraulic head h_{i-1}, at instant t_{i-1}, i.e., applying instead of Criterion 7.6 the criterion

$$h_i = \hat{h}_i \tag{7.13}$$

Then the effective transmissivity $\hat{T}_{i-1,i}$ can be obtained straightforward from Eq. 7.10 or by equalizing the hydraulic heads presented by Eqs. 7.7 and 7.8:

$$\hat{T}_{i-1,i} = -\frac{h_{i-1}}{1 - 2h_{i-1}} T_1 + \frac{1 - h_{i-1}}{1 - 2h_{i-1}} T_2 \tag{7.14}$$

The affecting factors for the transforming mechanism presented by Eq. 7.14 are

$$w_{1,i} = -\frac{h_{i-1}}{1 - 2h_{i-1}}, \quad w_{2,i} = \frac{1 - h_{i-1}}{1 - 2h_{i-1}} \tag{7.15}$$

It follows from the Expressions 7.15, that the effective hydraulic conductivity $\hat{T}_{i-1,i}$ is not a statistics. Note that, the affecting factors and the effective hydraulic transmissivity are not defined for the instant when the hydraulic head h_{i-1} is equal

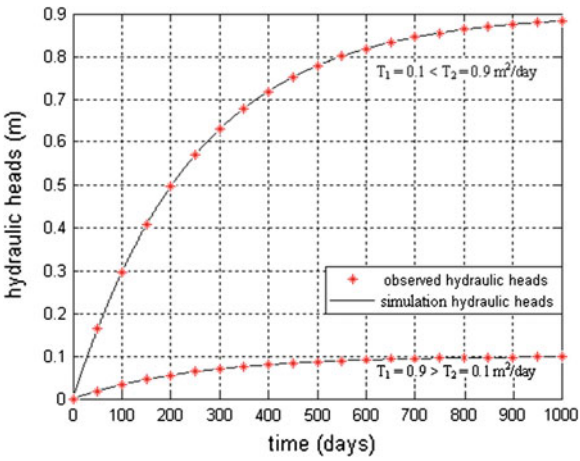

Fig. 7.3 Comparison of hydraulic heads obtained for a two-body object and a homogeneous simulation model

to 0.5 m. Note also that at $t = 0$ the hydraulic head $h(0) = h_0 = 0$. Thus factor $w_{1,1} = 0$ and the effective hydraulic transmissivity $\widehat{T}_{0.1} = T_2$.

The simulation results for two contrasting cases are presented in Fig. 7.3: one is the real world consisting of two bodies with the hydraulic transmissivities $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day and the other with the hydraulic transmissivities $T_1 = 0.9$ and $T_2 = 0.1$ m^2/day. The main distinction between these cases is that in one of them the asymptotic value of the 'observed' hydraulic heads h is equal to 0.1 m. It does not reach the crucial number $h = 0.5$ m. In the other the asymptote of the hydraulic heads is equal to 0.9 m, and the observed hydraulic heads overcome the crucial number $h = 0.5$ m.

Case 7.2.1 $T_1 = 0.9$ and $T_2 = 0.1$ m^2/day. The homogeneous model works perfectly. The affecting factors $w_{1,i}$ and $w_{2,i}$ and the effective transmissivity $\hat{T}_{i-1,i}$, are presented in Fig. 7.4.

The upper left effective hydraulic transmissivity value is equal to $T_2 = 0.1$ m^2/day which follows from Eqs. 7.14 and 7.15. The case demonstrates as well that the effective hydraulic transmissivities are incorrect geologically either, approaching zero with the time progress.

Case 7.2.2 $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day. The results are presented in Figs. 7.5 and 7.6. (The affecting factor $w_{1,i}$ is shown only, since $w_{2,i} = 1 - w_{1,i}$). In this case there exists the instant $t_{0.5}$ such that $h(t_{0.5}) = 0.5$ m. At this instant the affecting factors and the effective hydraulic transmissivity do not exist. Thus, the effective transmissivity is deprived of both physical and geological meanings in this case as well. But it does not preclude its values from providing effective reproduction of real world hydraulic heads.

As stated in Sect. 4.3, calibrating homogeneous models in a transient regime can permit the simulation results fitting the observations satisfactory for some short time interval. The use of the changing in time effective hydraulic

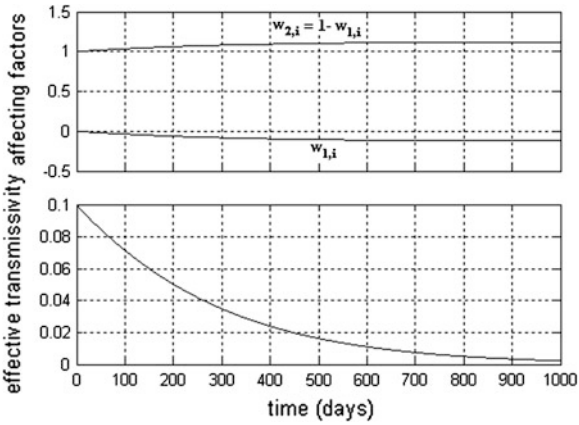

Fig. 7.4 Case 7.2.1: resulting affecting factors and effective hydraulic transmissivity

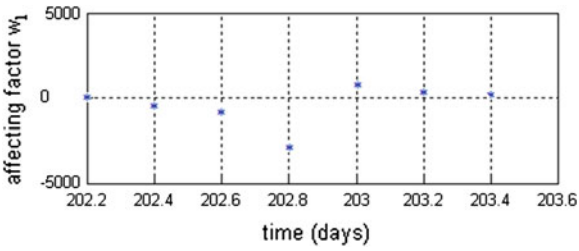

Fig. 7.5 Case 7.2.2: affecting factor $w_{1,i}$ in vicinity of the crucial instant $t_{0.5}$

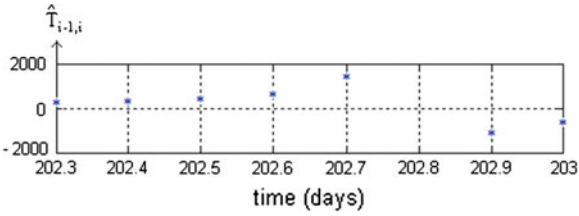

Fig. 7.6 Case 7.2.2: effective hydraulic transmissivity $\hat{T}_{i-1,i}$ in vicinity of the crucial instant $t_{0.5}$

transmissivity and conductivities permit obtaining considerably more accurate results. Two above cases demonstrate clearly those effective parameters are not statistics and even not geological or hydrogeological entities. They are just optimal characteristics of the corresponding systems and have not any physical meaning.

7.3 Implicit Numerical Simulation

In the previous section an explicit finite difference method is applied. To provide stability of the explicit numerical integration, the time increment Δt must be sufficiently small. The increment Δt equal to 0.1 day in Cases 7.2.1 and 7.2.2 is

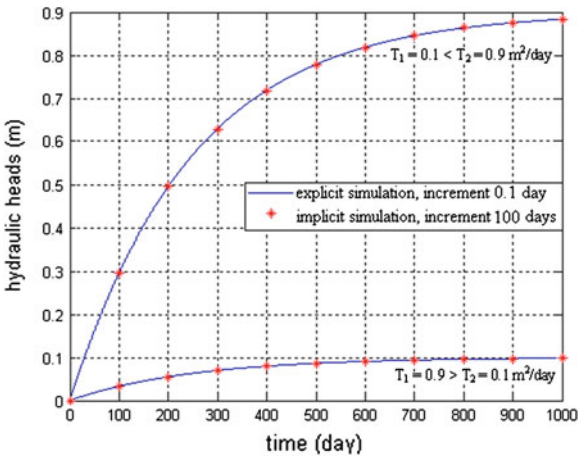

Fig. 7.7 Comparison of the explicit and implicit simulations

selected for this reason. Although at the present time of automation, duration of the time increment between measurements is not an issue, it may be not practical to have it very small. The stable numerical solution for the problem formulated in Sect. 7.1 can be obtained for time increments of an arbitrary duration by integrating Eq. 7.7 over time. Indeed for infinitesimal Δt ($\Delta t \to 0$), Eq. 7.7 can be rewritten, after separation of variables, as

$$\frac{dh}{(1-h)T_2 - hT_1} = \frac{dt}{SL^2}$$

Integrating the above equation in intervals $[h_{i-1}, h_i]$ and $[t_{i-1}, t_i]$ correspondingly yields

$$\int_{h_{i-1}}^{h_i} \frac{dh}{T_2 - (T_1 + T_2)h} = -\frac{1}{(T_1 + T_2)} \ln(T_2 - (T_1 + T_2)h)\Big|_{h_{i-1}}^{h_i} = \int_{t_{i-1}}^{t_i} \frac{dt}{SL^2} \quad (7.16)$$

It follows from Expressions 7.16 (see Box 7.1) that

$$h_i = \frac{T_2}{T_1 + T_2}\left\{1 - \left[1 - \left(\frac{T_1 + T_2}{T_2}\right)h_{i-1}\right] \exp\left(-\frac{T_1 + T_2}{SL^2}(t_i - t_{i-1})\right)\right\} \quad (7.17)$$

Comparison of the results obtained by Eqs. 7.7 and 7.17 are presented in Figs. 7.7 and 7.8 (the time increments for Eq. 7.17 are 100 days in Fig. 7.7 and 250 days in Fig. 7.8). In spite of increase of the time increment in 1,000 and 2,500 times, the results are identical.

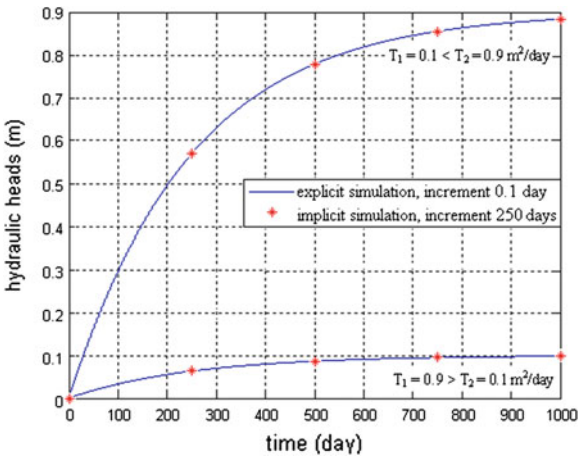

Fig. 7.8 Comparison of the explicit and implicit simulations

Text box 7.1
Inference of Eq. 7.17

Substituting in the right Equality of Expressions 7.16 the limits of integration yields

$$\frac{1}{(T_1+T_2)}\ln(T_2-(T_1+T_2)h)\Big|_{h_{i-1}}^{h_i} = -\frac{1}{(T_1+T_2)}\ln\frac{T_2-(T_1+T_2)h_i}{T_2-(T_1+T_2)h_{i-1}} = \frac{t_i-t_{i-1}}{SL^2}$$

Potentiating the above equality gives

$$\frac{T_2-(T_1+T_2)h_i}{T_2-(T_1+T_2)h_{i-1}} = \exp\left(-(T_1+T_2)\left(\frac{t_i-t_{i-1}}{SL^2}\right)\right)$$

or

$$T_2-(T_1+T_2)h_i = (T_2-(T_1+T_2)h_{i-1})\exp\left(-(T_1+T_2)\left(\frac{t_i-t_{i-1}}{SL^2}\right)\right)$$

Solving the above equation gives

$$h_i = \frac{T_2}{T_1+T_2} - \left(\frac{T_2}{T_1+T_2}-h_{i-1}\right)\exp\left(-(T_1+T_2)\left(\frac{t_i-t_{i-1}}{SL^2}\right)\right)$$

Factoring out the term T_2/T_1+T_2 yields Eq. 7.17.

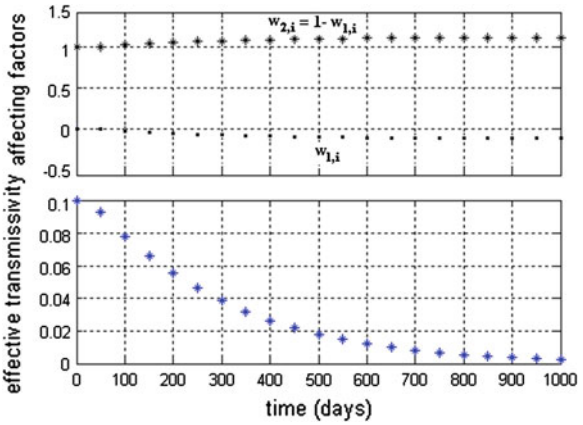

Fig. 7.9 Affecting factors and effective hydraulic transmissivity $\hat{T}_{i-1,i}$: $T_1 = 0.9$ and $T_2 = 0.1$ m^2/day

For an homogeneous simulation model $\left(T_1 = T_2 = \hat{T}_{i-1,i}\right)$, Eq. 7.17 converts into

$$\hat{h}_i = \frac{1}{2}\left(1 - (1 - 2h_{i-1})\ exp\left(-\frac{2\hat{T}_{i-1,i}}{SL^2}(t_i - t_{i-1})\right)\right) \tag{7.18}$$

The requirement to the model to be effective in the sense that $\hat{h}_i = h_i$ leads to the following choice for the effective hydraulic transmissivity

$$\hat{T}_{i-1,i} = \frac{SL^2}{2(t_i - t_{i-1})} \ln \frac{1 - 2h_{i-1}}{1 - 2h_i} \tag{7.19}$$

Substituting in Eq. 7.19 the hydraulic head h_i from Eq. 7.17 yields the following transforming mechanism

$$\hat{T}_{i-1,i} = \frac{SL^2}{2(t_i - t_{i-1})} \ln \frac{1 - 2h_{i-1}}{1 - \frac{2}{T_1+T_2}\left\{T_2 - [T_2 - (T_1 + T_2)h_{i-1}] \exp\left(-\frac{T_1+T_2}{SL^2}(t_i - t_{i-1})\right)\right\}} \tag{7.20}$$

The nonlinear transforming mechanism presented by Eq. 7.20 is difficult for analysis. However, it follows immediately from Eqs. 7.19 and 7.20 that the effective hydraulic transmissivity and the affecting factors are not defined for the case $T_1 < T_2$ at instant $t_{0.5}$ for which $h\ (t_{0.5}, L) = 0.5$ m. To the left and right from this instant the effective hydraulic transmissivities and the affecting factors are continuous function of time and the hydraulic transmissivities T_1 and T_2. The hydraulic head $h\ (t_{0.5}, L) < 0.5$ m always if $T_1 > T_2$, So, the effective transmissivity and the affecting are continuous in time in this case.

The affecting factors and the effective transmissivity for cases $T_1 = 0.9$ and $T_2 = 0.1$ m^2/day and $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day with the time increment

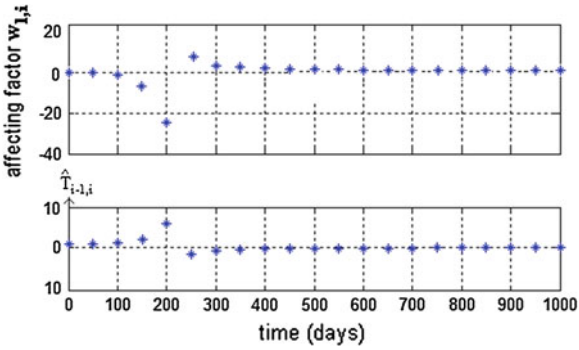

Fig. 7.10 Affecting factor $w_{1,i}$ and effective hydraulic transmissivity $\hat{T}_{i-1,i}$: $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day

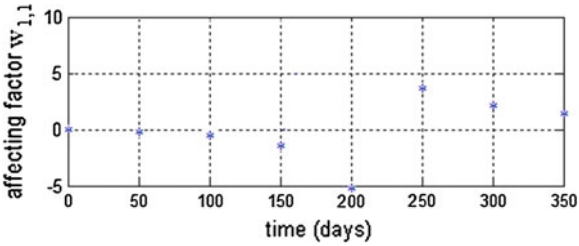

Fig. 7.11 $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day: affecting factors $w_{1,i}$

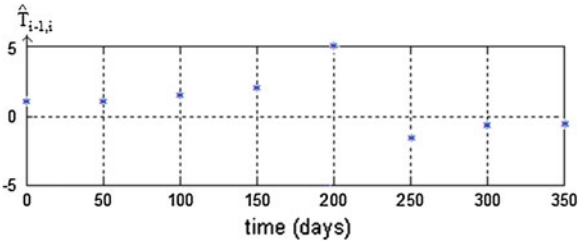

Fig. 7.12 $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day: effective hydraulic transmissivity

50 days are presented in Figs. 7.9 and 7.10. As expected, in the first case ($T_1 = 0.9$ and $T_2 = 0.1$ m^2/day) the affecting factors and the effective transmissivity are changing smoothly in time. The affecting factor $w_{1,i}$ takes non-positive values. The factor $w_{2,i}$ always exceeds 1. The effective hydraulic transmissivity decreases smoothly from 0.1 to 0. In the case $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day the affecting factors and the effective transmissivity are not defined in vicinity of instant approximately 200 days (Figs. 7.10, 7.11 and 7.12). Factually there exist two different transforming mechanisms. One is valid for time interval [0, 200] the other for interval ($\sim$200, 1000] days. It should be noted also that the affecting factors and the effective transmissivities obtained implicitly vary less than those obtained explicitly.

Sections 7.2 and 7.3 demonstrate that values of the effective parameters and the transforming mechanisms depend on the methods of their evaluation. Although some affecting factors of the mechanisms are negative, they are summing to one. Thus summing the affecting factors to one does not warrant that the pertinent effective parameter is a statistics. The most right values of the effective hydraulic transmissivity have zero as an asymptote. It occurs because the hydraulic head approaches asymptotically its maximum value at $x = L$.

Most hydrogeologists hold that the use of the effective but incorrect values of the geological parameter such as negative hydraulic conductivity or transmissivity in simulations is unacceptable. The question is what do we want: more accurate predictions and evaluations provided by physically incorrect parameters or less accurate ones based on physically correct parameters? The physically correct parameters can be incorrect geologically as demonstrated here as well as in Chap. 6. Why is the use of geologically incorrect parameters acceptable? Just because we do not know that they are incorrect? Being an engineer, I prefer the accuracy and the tools providing it. One must simply understand the systematic, optimizing, nature of the effective model parameters. They are not physical entities and are effective only in the formulation in which they have been obtained. Any change in a simulation problem changes the system and requires reevaluating the parameters. Applying the effective parameters obtained for one simulation problem to another can cause misleading results even when differences in the problem formulations may not seem to be considerable.

Chapter 8
Evaluation of Transforming Mechanisms

In the examples of Chaps. 6 and 7 the transforming mechanisms were obtained analytically. Such a direct approach can be cumbersome and even not available in many situations. The *two-level modeling* introduced below is more universal and seems to be more practical.

8.1 Two-Level Modeling Concept

The following hypothetical example explains the two-level modeling concept. Supposedly we are going to apply a particular simulation model to predict response of a particular geological object to a given impact. Information on the object is sparse, but we have complete information on many other geological sites with the same boundary conditions, impact and monitoring network. Their responses to the impact have been already observed. Applying our simulation model to those sites, we could evaluate how different geological conditions affect simulation results and use this knowledge. That is, we could see sensitivity of our model to different geological conditions, what parts and properties of geological objects (what information) are essential for effective predicting, applying our model, and how to assign its effective parameters. We could even abandon the model, if it is not satisfactorily effective and to try different ones.

In other words, we can accumulate specific engineering experience to deal with a specific problem. This does not eliminate the uncertainty of the simulation results, since the object of interest is not yet fully known. However, studies such as those would make our decisions related to predicting and its interpretation, including its uncertainty, more informed and focused. We acquire better understanding of what could go wrong and when, whether and when we have to update the simulation model, what additional feasible information could be necessary, etc.

Unfortunately, we do not have objects with completely known geological surroundings, exactly the same impacts, monitoring networks and long enough periods of observations. However, we can make them up as computer models. We can produce, using terminology of McLaughlin and Wood (1988), the synthetic

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
Springer Hydrogeology, DOI: 10.1007/978-3-319-03569-7_8,

data, reference systems, real worlds, as complex as computational resources permit, simulate their responses to a given impact, and compare those responses with the results yielded by a given simulation model. Simply speaking, we can make up some surrogate of the specific engineering experience.

There is nothing new about the use of artificial sites or synthetic data in groundwater modeling. In fact, the entire geostatistical approach with its made-up ensembles and other assumptions is based on them. McLaughlin and Wood (1988) use a synthetic, stochastically homogeneous ensemble of sites or, rather one site representing, as if, the mathematical expectation of the ensemble, to evaluate the accuracy of a proposed modeling study before extensive resources are committed to data collection and model development. Synthetic data are used by Zimmermann et al. (1998) and many others. Unfortunately, in practice the relationship between artificial and actual sites is ambiguous, and the extension of the obtained results to real world situations is difficult or even impossible (Eggleston et al. 1996).

The similarity of the reference systems to the geological object of interest is not necessary in the above hypothetical example. On the contrary, the diversity of conditions could be beneficial, permitting deeper understanding of the predictive problems. The reverse side of such diversity is the abundance of information making it difficult to review and analyze the acquired data. The transforming mechanisms are suggested as generalization of the obtained information.

Thus, the idea behind the described approach, called here two-level modeling, is to investigate how the given predictive model performs when representing more complex geological models. In a sense, it is Monte Carlo simulations, only reversed. Routinely in Monte Carlo simulations "the object of the investigation is a model itself" (Gentle 1985). Varying properties of a simulation model permits to explore the sensitivity of the simulation results to the model's parameters. However, the sensitivity of the simulation results to the model's parameters tells us nothing about the model's ability to represent the real geological objects (Two exceptions are possible: low or high sensitivity of a model indicate that it may not be practical). In two-level modeling the structure of the geological model is fixed and the real worlds vary. This permits evaluating how different factors, including the unknowns, can affect the simulation results.

The concept of the two-level modeling can be described in general on the example of Cases 6.2.1 and 6.2.2. The geological object, the real world, in these cases consists of four geological bodies and the geological model of two blocks. Pertinent transforming mechanisms for the first and second model blocks are described by equations

$$\begin{aligned} \hat{g}_1 &= w_{1,1}g_1 + w_{1,2}g_2 + w_{1,3}g_3 + w_{1,4}g_4 \\ \hat{g}_2 &= w_{2,1}g_1 + w_{2,2}g_2 + w_{2,3}g_3 + w_{2,4}g_4 \end{aligned} \tag{8.1}$$

where $\hat{g}_1 = 1/\hat{K}_1$ and $\hat{g}_2 = 1/\hat{K}_2$ are the effective specific hydraulic resistivities of the first and second model blocks ($\hat{K}_1$ and $\hat{K}_2$ are the corresponding effective hydraulic conductivities), $g_i = 1/K_i$ ($i = 1,\ldots, 4$) are the real world specific

Table 8.1 Set consisting of M subsets of observed effective and actual hydraulic resistivities

Effective parameters	Actual parameters
$\hat{g}_{1,1}$, $\hat{g}_{1,2}$	$g_{1,1}$, $g_{1,2}$, $g_{1,3}$, $g_{1,4}$
$\hat{g}_{2,1}$, $\hat{g}_{2,2}$	$g_{2,1}$, $g_{2,2}$, $g_{2,3}$, $g_{2,4}$
…	…
$\hat{g}_{m,1}$, $\hat{g}_{m,2}$	$g_{m,1}$, $g_{m,2}$, $g_{m,3}$, $g_{m,4}$
…	…
$\hat{g}_{M,1}$, $\hat{g}_{M,2}$	$g_{M,1}$, $g_{M,2}$, $g_{M,3}$, $g_{M,4}$

hydraulic resistivities of the geological bodies (K_i are the corresponding hydraulic conductivities).

The transforming mechanisms described by Eqs. 8.1 are linear and not depending on time. They can be interpreted as regressions and their affecting factors $w_{j,i}$ ($j = 1, 2$ and $i = 1,\ldots, 4$) as coefficients of those linear regressions. To evaluate them, we need a large enough set consisting of subsets of data: $\{g_{m,1}, g_{m,2}, g_{m,3}, g_{m,4}\}$ representing different real worlds and $\{\hat{g}_{m,1}, \hat{g}_{m,2}\}$ representing the corresponding effective parameters of the predictive model. M such subsets are presented in Table 8.1. Independent variables $\{g_{m,1}, g_{m,2}, g_{m,3}, g_{m,4}\}$ can be assigned arbitrarily, in particular to be generated as random values. Their knowledge permits calculating 'observations' (Eq. 6.7). The corresponding dependent variables $\{\hat{g}_{m,1}, \hat{g}_{m,2}\}$ for a given set $\{g_{m,1}, g_{m,2}, g_{m,3}, g_{m,4}\}$ can be calculated by solving System 6.10.

8.2 Examples of Evaluating Linear Transforming Mechanisms

Case 8.2.1 Let us come back to the problem described in Sect. 6.1: one-dimensional steady-state flow with constant recharge N to a fully penetrating trench at $X_0 = 0$ m in an unconfined aquifer on a horizontal aquitard (Fig. 8.1). The boundary conditions remain those assigned in Sect. 6.1.

As shown in Sect. 6.1, the effective resistivities for Cases 6.2.1 and 6.2.2 are solutions of System 6.10 which in the case of the uniform weighting ($p_1 = p_2 = p_3 = p_4 = 1$) takes form

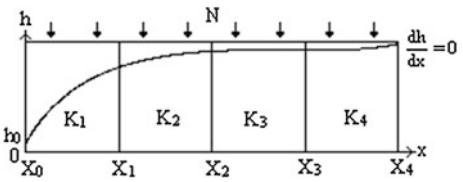

Fig. 8.1 One-dimensional steady-state flow to a fully-penetrating trench in an unconfined aquifer

$$\hat{g}_1 = 0.5635\left(h_1^2 - h_0^2\right) + 0.9659\left(h_2^2 - h_0^2\right) + 0.1546\left(h_3^2 - h_0^2\right) - 0.1159\left(h_4^2 - h_0^2\right)$$
$$\hat{g}_2 = -1.8931\left(h_1^2 - h_0^2\right) - 3.2454\left(h_2^2 - h_0^2\right) + 1.4005\left(h_3^2 - h_0^2\right) + 2.9491\left(h_4^2 - h_0^2\right). \tag{8.2}$$

Equation 8.2 permit evaluating effective values $\hat{g}_{1,m}$ and $\hat{g}_{2,m}$ for any subset m of the real world hydraulic resistivities $g_{m,1}$, $g_{m,2}$, $g_{m,3}$, $g_{m,4}$, if corresponding squared thicknesses of the aquifer are known (calculated by Eq. 6.7).

M such subsets are presented in Table 8.1. Equations 8.1 can be rewritten for convenience as one equation

$$\hat{g}_{m,j} = w_{j,1}g_{m,1} + w_{j,2}g_{m,2} + w_{j,3}g_{m,3} + w_{j,4}g_{m,4}, \quad j = 1, 2 \tag{8.3}$$

where index j defines the model block and $g_{m,1}$, $g_{m,2}$, $g_{m,3}$, $g_{m,4}$ are the randomly assigned hydraulic resistivities. Since the affecting factors $w_{j,1}$, $w_{j,2}$, $w_{j,3}$, $w_{j,4}$ of the linear transforming mechanisms do not depend on the real world hydraulic resistivities, they can be interpreted as regression coefficients of the regression represented by Eq. 8.3, and evaluated by the standard least squares technique, that is, by minimizing sum

$$s_j = \sum_{m=1}^{M} \left(w_{j,1}g_{m,1} + w_{j,2}g_{m,2} + w_{j,3}g_{m,3} + w_{j,4}g_{m,4} - \hat{g}_{m,j}\right)^2 \quad j = 1, 2 \tag{8.4}$$

where M is the number of sets $\{g_{m,1:4}\}$. The least squares technique leads to two systems ($j = 1, 2$) of linear equations for finding coefficients $w_{j,1}$, $w_{j,2}$, $w_{j,3}$, $w_{j,4}$:

$$\begin{aligned}
w_{j,1}\sum_{m=1}^{M} g_{m,1}^2 + w_{j,2}\sum_{m=1}^{M} g_{m,1}g_{m,2} + w_{j,3}\sum_{m=1}^{M} g_{m,1}g_{m,3} + w_{j,4}\sum_{m=1}^{M} g_{m,1}g_{m,4} &= \sum_{m=1}^{M} g_{m,1}\hat{g}_{m,j} \\
w_{j,1}\sum_{m=1}^{M} g_{m,1}g_{m,2} + w_{j,2}\sum_{i=1}^{M} g_{m,2}^2 + w_{j,3}\sum_{i=1}^{M} g_{m,2}g_{m,3} + w_{j,4}\sum_{i=1}^{M} g_{m,2}g_{m,4} &= \sum_{i=1}^{M} g_{m,2}\hat{g}_{m,j} \\
w_{j,1}\sum_{m=1}^{M} g_{m,1}g_{m,3} + w_{j,2}\sum_{i=1}^{M} g_{m,2}g_{m,3} + w_{j,3}\sum_{i=1}^{M} g_{m,3}^2 + w_{j,4}\sum_{i=1}^{M} g_{m,3}g_{m,4} &= \sum_{i=1}^{M} g_{m,3}\hat{g}_{m,j} \\
w_{j,1}\sum_{m=1}^{M} g_{m,1}g_{m,4} + w_{j,2}\sum_{i=1}^{M} g_{m,2}g_{m,4} + w_{j,3}\sum_{i=1}^{M} g_{m,3}g_{m,4} + w_{j,4}\sum_{i=1}^{M} g_{m,4}^2 &= \sum_{i=1}^{M} g_{m,4}\hat{g}_{m,j}.
\end{aligned} \tag{8.5}$$

Solving Systems 8.5 yields the affecting factors $w_{j,1}$, $w_{j,2}$, $w_{j,3}$, $w_{j,4}$.

The resulting transforming mechanisms obtained with $M = 50$, 100, 1,000 are exactly those obtained analytically for Cases 6.2.1 and 6.2.2 (Eq. 6.16):

$$\begin{aligned}
\hat{g}_1 &= 0.6861g_1 + 0.3139g_2 + 0.0072g_3 - 0.0072g_4 \\
\hat{g}_2 &= -0.3451g_1 + 0.3451g_2 + 0.8155g_3 + 0.1845g_4.
\end{aligned} \tag{8.6}$$

Case 8.2.2 Let us consider the above example only with more complex piecewise homogeneous real world. It comprises eight geological bodies with the boundaries at locations $X_0 = 0$, $X_1 = 12.5$, $X_2 = 25$, $X_3 = 37.5$, $X_4 = 50$, $X_5 = 62.5$, $X_6 = 75$, $X_7 = 87.5$ and $X_8 = 100$ m. The hydraulic conductivities K_i are constant within intervals $[X_{i-1}, X_i]$: K_1, K_2, K_3, K_4, K_5, K_6, K_7, K_8. The two block geological model with the boundary between the homogeneous blocks at $X_4 = 50$. The monitoring network located at the same four locations: $X_2 = 25$, $X_4 = 50$, $X_6 = 75$, and $X_8 = 100$ m. The criterion of efficiency remains the same, Eq. 6.6. Under assumption of uniform weighting of observations, it can be rewritten as

$$s = \sum_{i=1}^{4} \left(\hat{h}_{2i}^2 - h_{2i}^2 \right)^2. \tag{8.7}$$

Equation 6.4 for calculation of the real world observed squared water table elevations at the boundaries of geological bodies takes form

$$h_i^2 = h_{i-1}^2 + \frac{N}{K_i}(2X_8 - X_i - X_{i-1})(X_i - X_{i-1}), \quad i = 1, \ldots, 8 \tag{8.8}$$

The following equations describe 'the observations' at locations X_i (i = 1–8) for $N = 0.0001$ m/day ($g_i = 1/K_i$):

$$\begin{aligned}
h_1^2 &= h_0^2 + 0.2344 g_1 \\
h_2^2 &= h_0^2 + 0.2344 g_1 + 0.2031 g_2 \\
h_3^2 &= h_0^2 + 0.2344 g_1 + 0.2031 g_2 + 0.1719 g_3 \\
h_4^2 &= h_0^2 + 0.2344 g_1 + 0.2031 g_2 + 0.1719 g_3 + 0.1406 g_4 \\
h_5^2 &= h_0^2 + 0.2344 g_1 + 0.2031 g_2 + 0.1719 g_3 + 0.1406 g_4 + 0.1094 g_5 \\
h_6^2 &= h_0^2 + 0.2344 g_1 + 0.2031 g_2 + 0.1719 g_3 + 0.1406 g_4 + 0.1094 g_5 + 0.0781 g_6 \\
h_7^2 &= h_0^2 + 0.2344 g_1 + 0.2031 g_2 + 0.1719 g_3 + 0.1406 g_4 + 0.1094 g_5 + 0.0781 g_6 \\
&\quad + 0.0469 g_7 \\
h_8^2 &= h_0^2 + 0.2344 g_1 + 0.2031 g_2 + 0.1719 g_3 + 0.1406 g_4 + 0.1094 g_5 + 0.0781 g_6 \\
&\quad + 0.0469 g_7 + 0.0156 g_8.
\end{aligned} \tag{8.9}$$

Since the simulation model, the observation network and the criterion of goodness of fit stay the same, finding the effective hydraulic resistivities needs only change in enumeration of the observations in Eq. 8.2:

$$\begin{aligned}
\hat{g}_1 &= 0.5635\left(h_2^2 - h_0^2\right) + 0.9659\left(h_4^2 - h_0^2\right) + 0.1546\left(h_6^2 - h_0^2\right) - 0.1159\left(h_8^2 - h_0^2\right) \\
\hat{g}_2 &= -1.8931\left(h_2^2 - h_0^2\right) - 3.2454\left(h_4^2 - h_0^2\right) + 1.4005\left(h_6^2 - h_0^2\right) + 2.9491\left(h_8^2 - h_0^2\right).
\end{aligned} \tag{8.10}$$

The regression equations relating the real world hydraulic resistivities and the effective hydraulic conductivities of two model blocks differ from Eq. 8.1 by the numbers of the independent variables g_i and the regressions coefficients $w_{1,i}$ and $w_{2,i}$ representing the affecting factors:

$$\begin{aligned}\hat{g}_1 &= w_{1,1}g_1 + w_{1,2}g_2 + w_{1,3}g_3 + w_{1,4}g_4 + w_{1,5}g_5 + w_{1,6}g_6 + w_{1,7}g_7 + w_{1,8}g_8\\ \hat{g}_2 &= w_{2,1}g_1 + w_{2,2}g_2 + w_{2,3}g_3 + w_{2,4}g_4 + w_{2,5}g_5 + w_{2,6}g_6 + w_{2,7}g_7 + w_{2,8}g_8.\end{aligned} \tag{8.11}$$

The standard least squares technique applied for evaluating the affecting factors leads to two linear systems consisting of the equation including eight regression coefficients each. Generating randomly the real worlds data $g_{m,1}$, $g_{m,2}$, $g_{m,3}$, $g_{m,4}$, $g_{m,5}$, $g_{m,6}$, $g_{m,7}$, $g_{m,8}$, permits calculating the squared water table elevations $h^2_{m,2}$, $h^2_{m,4}$, $h^2_{m,6}$, and $h^2_{m,8}$, the effective hydraulic conductivities $\hat{g}_{m,j}$ and finally the affecting factors $w_{j,1}$, $w_{j,2}$, $w_{j,3}$, $w_{j,4}$, $w_{j,5}$, $w_{j,6}$, $w_{j,7}$, $w_{j,8}$. For the situation corresponding to Cases 6.2.1 and 6.2.2 and the 'real world' consisting of eight geological bodies the results are transforming mechanisms

$$\begin{aligned}\hat{g}_1 =& 0.3676g_1 + 0.3185g_2 + 0.1727g_3 + 0.1413g_4 + 0.0042g_5\\ &+ 0.0030g_6 - 0.0054g_7 - 0.0018g_8\\ \hat{g}_2 =& -0.1849g_1 - 0.1602g_2 + 0.1899g_3 + 0.1553g_4 + 0.4759g_5\\ &+ 0.3397g_6 + 0.1383g_7 + 0.0461g_8.\end{aligned} \tag{8.12}$$

The mechanisms described by Eq. 8.12 have the properties of the transforming mechanisms described by Eqs. 5.5 and 5.6. Indeed, the affecting factors belonging to the evaluated blocks $w_{1,1}$, $w_{1,2}$, $w_{1,3}$, $w_{1,4}$ and $w_{2,5}$, $w_{2,6}$, $w_{2,7}$, $w_{2,8}$ sum to one and the affecting factors belonging to the affecting blocks $w_{1,5}$, $w_{1,6}$, $w_{1,7}$, $w_{1,8}$ and $w_{2,1}$, $w_{2,2}$, $w_{2,3}$, $w_{2,4}$ are sum to zero. Besides, the affecting factors are additive. Thus, if $K_1 = K_2$, $K_3 = K_4$, $K_5 = K_6$, $K_7 = K_8$, Eq. 8.12 convert into Eq. 8.5.

Properties 1 and 2 of the transforming mechanisms (Sect. 5.3) permit simplification of the evaluating of the affecting factors be decreasing their numbers. For example, Regressions 8.1 can be rewritten as

$$\begin{aligned}w_{1,1}(g_1 - g_2) + w_{1,3}(g_3 - g_4) &= \hat{g}_1 - g_2\\ w_{2,1}(g_1 - g_2) + w_{2,3}(g_3 - g_4) &= \hat{g}_2 - g_4.\end{aligned} \tag{8.13}$$

Applying the least squares method to the first Eq. 8.13 leads to system of two equations for evaluating $w_{1,1}$ ($w_{1,2} = 1 - w_{1,1}$) and $w_{1,3}$ ($w_{1,4} = -w_{1,3}$). The second equation yields system of two equation for evaluating $w_{2,1}$ ($w_{2,2} = -w_{2,1}$) and $w_{2,3}$ ($w_{2,4} = 1 - w_{2,3}$).

8.3 Transforming Mechanisms for Effective Recharge Rates at Borden Landfill

Let us come back to the problem described in Sect. 6.4. The mechanism converting three recharge rates in the effective recharge of a homogeneous model simulating the water table within the Borden site was obtained analytically there. To this end, the available observations on the streamline starting at $x = 300$ m and the aquifer base elevations are used. The effective recharge rate $\hat{N}$ has been calculated, using additionally the water table elevation providing satisfactory reproduction of the streamline and the arrival time. Here the transforming mechanism is evaluated by two-level modeling. The technique applied is exactly as described in the above section.

This time the goal is to obtain the affecting factors (w_1, w_2, and w_3) of the transforming mechanism

$$\hat{N} = w_1 N_3 + w_2 N_4 + w_3 N_5 \tag{8.14}$$

where $\hat{N}$ is the effective recharge rate of the homogeneous model and N_3, N_4, N_5 are the actual recharge rates (Fig. 8.2). For subset m of the independent variables N_3, N_4, N_5, Relationship 8.14 takes form

$$\hat{N}_m = w_1 N_{m,3} + w_2 N_{m,4} + w_3 N_{m,5}. \tag{8.15}$$

Equation 8.15 can be interpreted as linear regression in which the affecting factors w_1, w_2, w_3 can be evaluated as regression coefficients. Thus first, M sets of recharge patterns $\{N_{3:5}\}$ and corresponding to them M sets of the effective recharge rates $\left\{\hat{N}\right\}$ should be accumulated (M must be a large enough number). Then the redundant system of equations like Eq. 8.15 can be made up and solved for the affecting factors w_1, w_2, w_3 by the least squares method.

Subsets $\{N_{m,3}, N_{m,4}, N_{m,5}\}$ can be generated randomly. The problem is evaluating the recharge rate $\hat{N}_m$ providing effective reproducing the water table. The effective recharge rates should be obtained based on the generated recharge rate $\{N_{m,3}, N_{m,4}, N_{m,5}\}$ and data presented in Table 8.2. Since the randomly picked

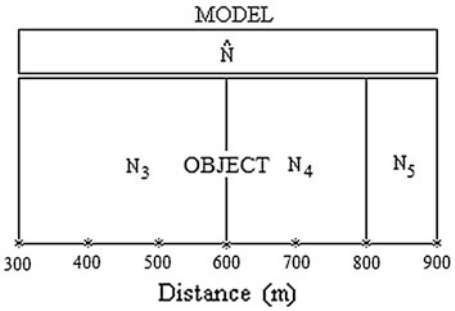

Fig. 8.2 Borden site and its homogeneous model with respect to the recharge rate

Table 8.2 Data for evaluating effective recharge rate $\hat{N}_m$

#	x	H_S	Y	$u = H_S - Y$	Q_m	$\hat{Q}_m$
0	300	222.31	204.31	17.99	Q_S	Q_S
1	400	219.25	206.17	13.08	$Q_S + 100N_{m,3}$	$Q_S + 100\hat{N}_m$
2	500	218.26	209.55	8.71	$Q_S + 200N_{m,3}$	$Q_S + 200\hat{N}_m$
3	600	217.46	210.85	6.61	$Q_S + 300N_{m,3}$	$Q_S + 300\hat{N}_m$
4	700	216.07	211.33	4.74	$Q_S + 300N_{m,3} + 100N_{m,4}$	$Q_S + 400\hat{N}_m$
5	800	215.47	211.86	3.61	$Q_S + 300N_{m,3} + 200N_{m,4}$	$Q_S + 500\hat{N}_m$
6	900	215.67	212.79	2.88	$Q_S + 300N_{m,3} + 200N_{m,4} + 100N_{m,5}$	$Q_S + 600\hat{N}_m$

recharge rates $\{N_{m,3}, N_{m,4}, N_{m,5}\}$ are known, there is no need to resort to, as if, steady-state water table and its effective simulation (Eqs. 6.32, 6.33). So the effective recharge $\hat{N}_m$ can be evaluated by minimization of Criterion 6.36 which, for working with subsets $\{N_{m,3}, N_{m,4}, N_{m,5}\}$ and $\hat{N}_m$, can be rewritten as

$$s_m = \sum_{i=1}^{6} \left(\left(\hat{Q}_{m,i} - Q_{m,i} \right) \left(H_{S,i} - Y_i \right) \right)^2. \tag{8.16}$$

The standard least squares technique lead to equation

$$\begin{aligned} \left(u_1^2 + 4u_2^2 + 9u_3^2 + 16u_4^2 + 25u_5^2 + 36u_6^2 \right) \hat{N}_m = & \left(u_1^2 + 4u_2^2 + 9u_3^2 + 12u_4^2 + 15u_5^2 + 18u_6^2 \right) \\ & N_{m,3} + \left(4u_4^2 + 10u_5^2 + 12u_6^2 \right) N_{m,4} + 6u_6^2 N_{m,5}. \end{aligned} \tag{8.17}$$

So

$$\hat{N}_m = \frac{\left(u_1^2 + 4u_2^2 + 9u_3^2 + 12u_4^2 + 15u_5^2 + 18u_6^2 \right) N_{m,3} + \left(4u_4^2 + 10u_5^2 + 12u_6^2 \right) N_{m,4} + 6u_6^2 N_{m,5}}{u_1^2 + 4u_2^2 + 9u_3^2 + 16u_4^2 + 25u_5^2 + 36u_6^2}. \tag{8.18}$$

The coefficients in terms containing $N_{m,3:5}$ are made up from observations. They are equal to those presented in Eq. 6.37, though the corresponding effective recharges $\hat{N}_m$ are different. However, such convenience is not always available, and it can be easier to apply the two-level modeling exactly as this has been done in the previous section. The affecting factors w_1, w_2, w_3 are those minimizing sum

$$s = \sum_{m=1}^{M} \left(\hat{N}_m - w_1 N_{m,3} - w_2 N_{m,4} - w_3 N_{m,5} \right)^2. \tag{8.19}$$

The standard least squares technique leads to the following system of linear equations for evaluating the affecting factors:

$$
\begin{aligned}
w_1 \sum_{m=1}^{M} N_{m,3}^2 + w_2 \sum_{m=1}^{M} N_{m,3} N_{m,4} + w_3 \sum_{m=1}^{M} N_{m,3} N_{m,5} &= \sum_{m=1}^{M} N_{m,3} \hat{N}_m \\
w_1 \sum_{m=1}^{M} N_{m,4} N_{m,3} + w_2 \sum_{m=1}^{M} N_{m,4}^2 + w_3 \sum_{m=1}^{M} N_{m,4} N_{m,5} &= \sum_{m=1}^{M} N_{m,4} \hat{N}_m \\
w_1 \sum_{m=1}^{M} N_{m,5} N_{m,3} + w_2 \sum_{m=1}^{M} N_{m,5} N_{m,4} + w_3 \sum_{m=1}^{M} N_{m,5}^2 &= \sum_{m=1}^{M} N_{m,5} \hat{N}_m .
\end{aligned}
\tag{8.20}
$$

Solving System 8.20 yields the affecting factors $\{w_1, w_2, w_3\}$ which for M equal 10, 100 and 1,000 stay the same:

$$w_1 = 0.8005, \quad w_2 = 0.1727, \quad w_3 = 0.0269.$$

That is, the affecting factors are exactly those obtained in Sect. 6.4 (Eq. 6.37).

The explicit use of the properties of the transforming mechanism can simplify evaluating the affecting factors as shown in the previous section. In particular, since the affecting factors summing to one, one of them can be expressed through two others. So instead of system 8.20 consisting of three equations, it is possible to work with a system consisting of two equations.

It may seem that in the case of the linear transforming mechanisms the two-level modeling is more complicated than their analytical deducing in Chap. 6. However, when geological objects and the corresponding simulation model become more complex the situation may change. Besides the two-level modeling may work when there are no observed data yet, i.e. before starting field researches as shown in Sect. 8.2 or with the data whose accuracy is low as with the data on the water table in the Borden site. The procedures of the two-level modeling reveal more information on objects. They are easier to be standardized and programmed.

8.4 Two-Level Modeling for Non-Linear Transforming Mechanisms

The problems involving the non-linear transforming mechanisms are considerably more complex than those involving the linear mechanisms, since the non-linear mechanisms depend on the actual distributions of the actual properties (geological bodies). There is no developed methodology of their evaluation at this moment. However, some notions on how it could be done are demonstrated below on the conceptual examples of Sect. 7.3.

Let a two body geological object be simulated by a one-block model. To simulate effectively the hydraulic heads $h(L, t)$ under the boundary conditions: $h(0, t) = 0$ and $h(2L, t) = 1$, we have to use the effective hydraulic transmissivity varying in time. As shown in Sect. 7.3 the pertinent effective hydraulic conductivities are described by Eq. 7.19 which is repeated here:

$$\hat{T}_{i-1,i} = \frac{SL^2}{2\Delta t} \ln \frac{1 - 2h_{i-1}}{1 - 2h_i} \tag{8.21}$$

[$S = 0.1$ is the storativity, $h_{i-1} = h(L, t_{i-1})$ and $h_i = h(L, t_i)$ are the observed hydraulic heads at $L = 50$ m and instances $t_{i\text{-}1}$ and t_i]. Equation 8.21 permits evaluating the effective transmissivity $\hat{T}_{i-1,i}$ which reproduces exactly the hydraulic head h_i based on the known hydraulic head h_{i-1}. They are obtained for implicit formulation of the simulation problem and valid for the arbitrary time increment Δt between observations. In the example discussed below $\Delta t = t_i - t_{i-1}$ is equal to 7 days.

Equation 8.21 assumes that both hydraulic heads h_{i-1} and h_i are known. That is, Eq. 8.21 is a tool for calibration. As we know, the effective transmissivities depends on time. So the goal should be extrapolating them beyond the period of calibration. It is possible since, as follows from Eq. 8.21, the effective transmissivity is a continuous function of h_{i-1} and h_i, and consequently of time, besides the instant when one of them is equal 0.5 m in our case. For this reason, we can expect that the effective transmissivity evaluated by Eq. 8.21 remains close to efficiency for some time beyond the calibration period. As soon as monitoring revels that the simulation results become unsatisfactory, the simulation model must be recalibrated.

Case 8.4.1 The hydraulic transmissivity of the first body is greater than of the second one. (To make the 'observations', the transmissivity T_1 and T_2 are assigned equal to 0.9 and 0.1 m^2/day respectively in this case). The model has been calibrated on the available thirteen hydraulic heads obtained during first thirteen weeks (91 days) of observation. The results are presented in Fig. 8.3. The calibration is an obvious success. To extrapolate its results beyond the period of calibration we need to describe the time dependence of the effective transmissivity explicitly. It can be done in many ways. The approximation (regression) presented in Fig. 8.3 is polynomial of the third degree

$$\begin{aligned}\hat{T} \approx &- 1.0833 \times 10^{-10}(t - \bar{t})^3 + 3.7356 \times 10^{-7}(t - \bar{t})^2 \\ &- 2.8554 \times 10^{-4}(t - \bar{t}) + 0.0862\end{aligned} \tag{8.22}$$

where $\bar{t} = 49$ days.

During about 60 weeks (420 days) the model worked more than satisfactorily (Fig. 8.4).

Then a systematic deviation appears between the simulation results and the observations. If the deviations are not permissible, the model must be recalibrated based on all available data. Let the new approximation be a polynomial of the 4th order. The least squares method applied to the 81 weeks of 'observations' yields:

$$\begin{aligned}\hat{T} \approx &- 3 \times 10^{-14}(t - \bar{t})^4 - 2.0173 \times 10^{-10}(t - \bar{t})^3 \\ &+ 2.3536 \times 10^{-7}(t - \bar{t})^2 - 1.3809 \times 10^{-4}(t - \bar{t}) + 0.0372\end{aligned} \tag{8.23}$$

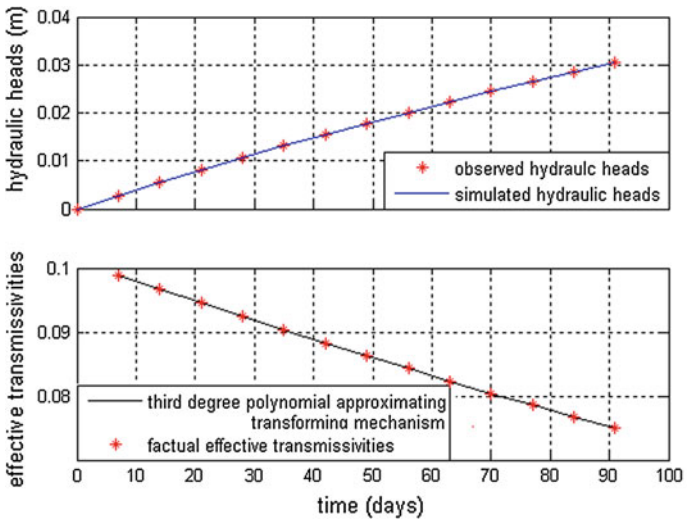

Fig. 8.3 Case 8.4.1: calibration on data related to the first 13 weeks

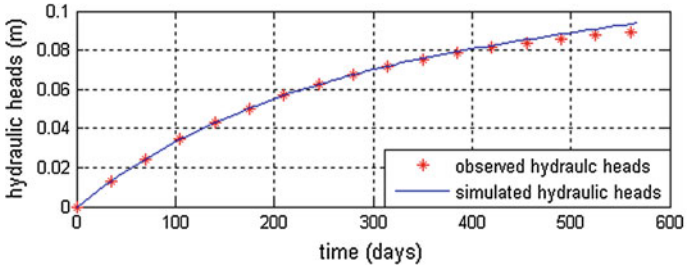

Fig. 8.4 Case 8.4.1: extrapolating simulations beyond period of calibration to the 81th week, applying the transforming mechanisms described by Eq. 8.22

where $\bar{t} = 287$ days. The results of recalibration and extrapolation the transforming mechanisms described by Eq. 8.23 on the entire prediction period, 1,000 days, are presented in Figs. 8.5 and 8.6. They reveal that there is no need in additional model recalibration.

By the way, location $x = 50$ m, convenient for illustration, is not the best for monitoring in this case. The hydraulic heads $h(L, t)$ is approaching the value 0.1 asymptotically. The closer the observed hydraulic heads to this value the less informative they become. To the right from that location, say, at $x = 75$ m, the process of development of the hydraulic heads is more dynamic and informative.

Case 8.4.2 The hydraulic transmissivity of the first body is less than the one of the second body. To make the "observations" $T_1 = 0.1$ and $T_2 = 0.9$ m^2/day are assigned in this case. The case differs from the previous one. Developing in time,

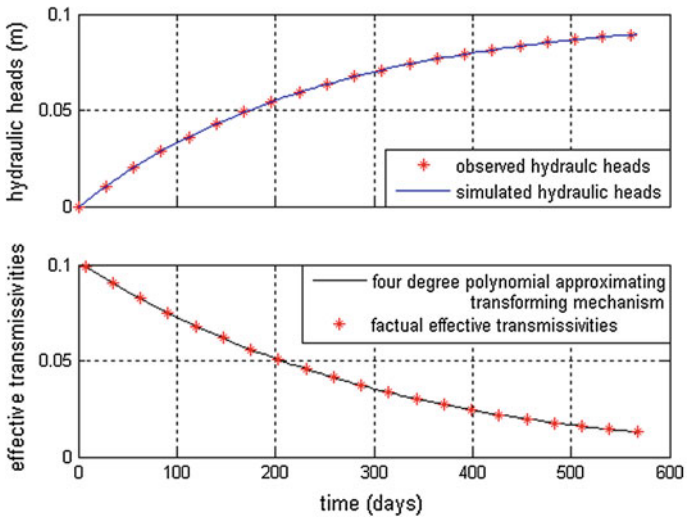

Fig. 8.5 Case 8.4.1: recalibration on data related to the first 81 weeks. The effective hydraulic transmissivity given by Eq. 8.23

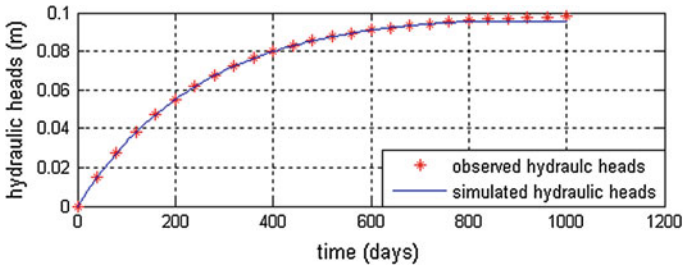

Fig. 8.6 Case 8.4.1: extrapolating simulations beyond period of calibration (81 weeks) applying the transforming mechanisms described by Eq. 8.23

the hydraulic heads exceed the critical value $h(L,\ t) = 0.5$ m. According to Eq. 8.21, the effective hydraulic transmissivity as a function of time is discontinuous at that instant. Thus, two different transforming mechanisms have to be applied for simulation: one for period when $h(L,\ t)$ is less than 0.5 m less and the other for the period when $h(L,\ t)$ exceeds 0.5 m.

The model has been calibrated on the available thirteen hydraulic heads obtained during first 13 weeks of observations. The results of calibration are presented in Fig. 8.7. They seem to be quite satisfactory. To extrapolate those results, on the hydraulic heads development beyond the period of calibration, we need to describe the time dependence of the effective transmissivity mathematically. The regression which does the job is presented by equation

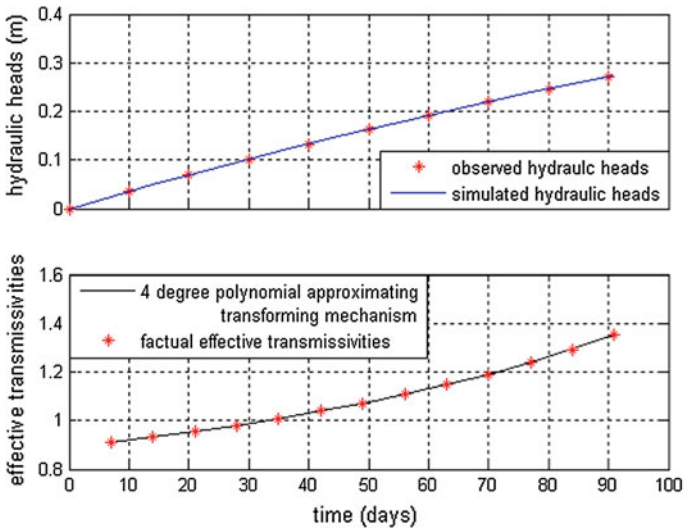

Fig. 8.7 Case 8.4.2: calibration on data related to the first 13 weeks

$$\begin{aligned}\hat{T} \approx & 1.4589 \times 10^{-9}(t-\bar{t})^4 + 2.2495 \times 10^{-7}(t-\bar{t})^3 \\ & + 3.2093 \times 10^{-5}(t-\bar{t})^2 + 4.8893 \times 10^{-3}(t-\bar{t}) + 1.0714\end{aligned} \tag{8.24}$$

where $\bar{t} = 49$ days. It works excellently on the first thirteen observations. Since it is continuous, we can try to extrapolate it for some further time. As shown in Fig. 8.8, it works satisfactory up to 28 weeks (196 days).

Since to this time the hydraulic head is nearing the critical number 0.5 m, it may have no sense to extrapolate the obtained transforming mechanism further. As soon as the hydraulic head exceeds the critical value, new data should be collected for new calibration. Let the collection start at the 30th week and last 13 weeks, that is, during period from 210 to 301 days. The results of the model calibration

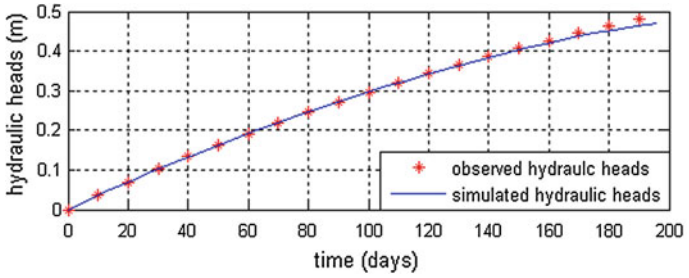

Fig. 8.8 Case 8.4.2: extrapolating simulations beyond period of calibration to the 28th week, applying the transforming mechanisms described by Eq. 8.24

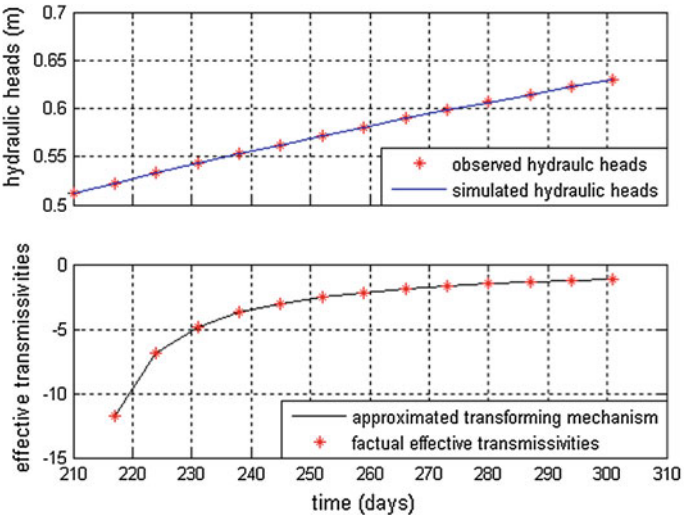

Fig. 8.9 Case 8.4.2: recalibration on data related to 30–43 weeks

are presented in Fig. 8.9 and seem to be satisfactory. The transforming mechanism in this case is presented by regression

$$\frac{1}{\tilde{T}} \approx -4.0923 \times 10^{-8}(t-\bar{t})^3 - 1.9219 \times 10^{-5}(t-\bar{t})^2 - 9.8878 \times 10^{-3}(t-\bar{t}) - 0.4697 \tag{8.25}$$

where $\bar{t} = 259$ days. This transforming mechanism was extrapolated on all remaining period of simulation for 30–143 weeks (about 1,000 days). As shown in Fig. 8.10, there is no need for the model recalibration.

Contrary to Case 8.4.1, location $L = 50$ m is not a bad choice for monitoring this object since the range of the hydraulic heads is larger in this case. The point

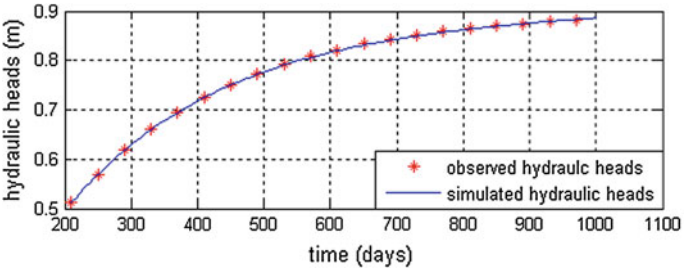

Fig. 8.10 Case 8.4.2 extrapolating simulations beyond period of calibration (43 weeks) applying the transforming mechanisms described by Eq. 8.25

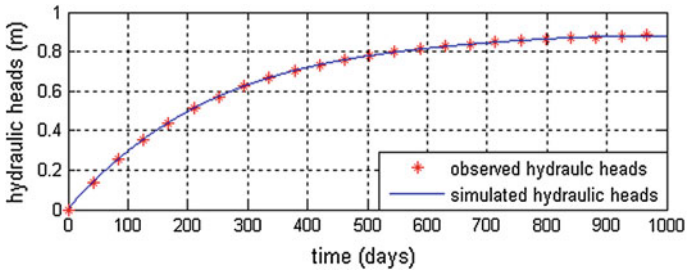

Fig. 8.11 Case 8.4.2: reproducing development hydraulic heads by Eq. 8.26 without involving effective hydraulic transmissivities

here is that assuming different values T_1 and T_2 or rather different ratios T_2/T_1, the choice for location or locations for monitoring wells can be done priory starting field explorations.

8.5 Conclusion

This chapter illustrates the general concept and demonstrates a principal possibility to evaluate the mechanisms transforming real properties of geological objects into the parameters which are effective in simulation of predictive or evaluating problems according to those problems' formulations. However, evaluating the non-linear transforming may require overcoming considerable computational difficulties.

Indeed, evaluation of the linear transforming mechanisms is straightforward. If a linear mechanism depends on time, the procedure described in Sects. 8.1 and 8.2 must be repeated for the instants of interest. However, it can be done before of the beginning of field exploration still. Evaluation of the non-linear mechanisms requires some knowledge on the object's reaction on the planning impact, that is, monitoring of the reaction, and recalibration model from time to time.

By the way, it is possible to predict the development of the hydraulic heads without finding effective parameters, transforming mechanisms, and physically based simulation models at all. The available observations can be used for evaluating the regression relationship describing those observations in time which can be extrapolated in future. When it becomes unsatisfactory, the additional data obtained by monitoring are applied to obtain new regression relationship, and so on. In particular, in Case 8.4.2, the regression (Fig. 8.11)

$$\begin{aligned}\hat{h} \approx &- 1.66 \times 10^{-12} t^4 + 4.9846 \times 10^{-9} t^3 \\ &- 5.8572 \times 10^{-6} t^2 + 0.0034 t\end{aligned} \tag{8.26}$$

works satisfactory.

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Chapter 9
Inverse Problems and Transforming Mechanisms

As mentioned in Chap. 4, the term 'inverse problem' is not a synonym of the terms 'model identification', 'model calibration', 'historical matching', 'site specific validation'. Those terms relate to evaluating the effective characteristics for a given simulation model which is usually an optimization problem. The goal of the inverse problems is to estimate the actual properties of geological objects using available observations on natural phenomena or on responses on man made impacts. Since the notions on geological objects are not more than models, it seems to be more accurate to define inverse problems as applications of simpler models for evaluating properties of more complex ones. The simpler models applied for solving inverse problems are called the *interpretation models*.

The physical and geological meaning of results of model identification does not matter. The effective parameters must provide the best results for the coupled simulation problem, and they depend on formulation of the problem. In contrast, the result of solving an inverse problem must not depend on its formulations, and its solution is not acceptable, if it is deprived of the physical meaning.

As demonstrated in Sect. 6.3, the linear transforming mechanisms obtained in Sect. 6.2 can be applied to solving inverse problems in a straightforward way. Indeed, if affecting factors $w_{j,i}$ (j = 1–2 indicates model blocks, i = 1–4 geological bodies) and the pertinent effective parameter $\hat{g}_j$ are known, a transforming mechanism

$$\hat{g}_j = w_{j,1}g_1 + w_{j,2}g_2 + w_{j,3}g_3 + w_{j,4}g_4 \tag{9.1}$$

can be considered as an equation with respect to the unknown actual property values $g_{1:4}$. So it suffices to make up the sufficient number of the transforming mechanisms with known affecting factors and effective parameters values, to consider them as a system of equations, closed or redundant, and to solve it for $g_{1:4}$. Exactly this has been done in Sect. 6.3, (System 6.24). However development of many different formulations of a model identification problem, like those in Sect. 6.2, is a cumbersome enterprise. The approach described in this chapter standardizes this procedure. The manifold of the mechanisms in this procedure is being created by automatic assigning different, random, sets of weights to the available observations.

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Inverse problems are incorrect inherently. However, as shown in Sect. 4.1, this does not mean that they are incorrect always. Mathematical correctness or incorrectness of an inverse problem depends on the actual structure and properties of the geological object, the choice of the model representing the object and the diversity and accuracy of the available observations. Any practicing geophysicist has the experience of success and failure, interpreting geophysical data. Understanding of the geology and the observed process are the necessary condition of the success.

9.1 Linear Transforming Mechanisms: Illustrative Examples

Let us rewrite Criterion 6.6, introducing arbitrary subsets of the weights $\{p\}_m = \{p_{m,1}\ p_{m,2},\ p_{m,3}\ p_{m,4}\}$ to the errors of our simulation of the squared thickness of the aquifer in different observation locations:

$$s_m = \sum_{i=1}^{4} p_{m,i}\left(\hat{h}_{p,i}^2 - h_i^2\right)^2. \tag{9.2}$$

Then System 6.10 converts into

$$\begin{aligned}
&\left(0.4375^2\, p_{m,1} + 0.75^2\left(p_{m,2} + p_{m,3} + p_{p,4}\right)\right)\hat{g}_{m,1} + 0.75\left(0.1875\, p_{m,3} + 0.25\, p_{m,4}\right)\hat{g}_{m,2} \\
&= 0.4375\, p_{m,1}\left(h_1^2 - h_0^2\right) + 0.75\left(p_{m,2}\left(h_2^2 - h_0^2\right) + p_{m,3}\left(h_3^2 - h_0^2\right) + p_{m,4}\left(h_4^2 - h_0^2\right)\right) \\
&0.75\left(0.1875\, p_{m,3} + 0.25\, p_{m,4}\right)\hat{g}_{p,1} + \left(0.1875^2 p_{m,3} + 0.25^2 p_{m,4}\right)\hat{g}_{m,2} \\
&= 0.1875\, p_{m,3}\left(h_3^2 - h_0^2\right) + 0.25\, p_{m,4}\left(h_4^2 - h_0^2\right).
\end{aligned} \tag{9.3}$$

The matrix of System 9.3 is

$$c_m = \begin{Bmatrix} 0.4375^2\, p_{m,1} + 0.75^2\left(p_{m,2} + p_{m,3} + p_{m,4}\right) & 0.75\left(0.1875\, p_{m,3} + 0.25\, p_{m,4}\right) \\ 0.75\left(0.1875\, p_{m,3} + 0.25\, p_{m,4}\right) & 0.1875^2\, p_{m,3} + 0.25^2\, p_{m,4} \end{Bmatrix}. \tag{9.4a}$$

Its right-hand term vector is

$$b_m = \begin{Bmatrix} 0.4375\, p_{m,1}\left(h_1^2 - h_0^2\right) + 0.75\left(p_{m,2}\left(h_2^2 - h_0^2\right) + p_{m,3}\left(h_3^2 - h_0^2\right) + p_{m,4}\left(h_4^2 - h_0^2\right)\right) \\ 0.1875\, p_{m,3}\left(h_3^2 - h_0^2\right) + 0.25\, p_{m,4}\left(h_4^2 - h_0^2\right) \end{Bmatrix}. \tag{9.4b}$$

(Compare to Expressions 6.11). Solving System 9.3 yields two values of the effective hydraulic resistivities: $\hat{g}_{2m-1}$ and $\hat{g}_{2m}$.

To find the affecting factors of the corresponding transforming mechanisms, Eq. 6.15 can be applied to each set of the weights:

$$\begin{aligned}\{w_{2m-1,1} \quad w_{2m-1,2} \quad w_{2m-1,3} \quad w_{2m-1,4}\} &= \left\{\frac{W_{2m-1}c_{m,2,2} - W_{2m}c_{m,1,2}}{c_{m,1,1}c_{m,2,2} - c_{m,1,2}c_{m,2,1}}\right\}' \\ \{w_{2m,1} \quad w_{2m,2} \quad w_{2m,3} \quad w_{2m,4}\} &= \left\{\frac{W_{2m,}c_{m,1,1} - W_{2m-1,1}c_{m,2,1}}{c_{m,1,1}c_{m,2,2} - c_{m,1,2}c_{m,2,1}}\right\}'\end{aligned} \tag{9.5}$$

where vectors W_{2m-1} and W_{2m} are defined by Expressions 6.14.

$$\begin{aligned}W_{2m-1} &= \left\{\begin{array}{c} 0.4375\left(0,4375\,p_{m,1} + 0.75\left(p_{m,2} + p_{m,3} + p_{m,4}\right)\right) \\ 0.3125 \times 0.75\left(p_{m,2} + p_{m,3} + p_{m,4}\right) \\ 0.1875 \times 0.75\left(p_{m,3} + p_{m,4}\right) \\ 0.75 \times 0.0625\,p_{p,4}\end{array}\right\} \\ W_{2m} &= \left\{\begin{array}{c} 0,4375\left(0.1875\,p_{m,3} + 0.25\,p_{m,4}\right) \\ 0.3125\left(0.1875\,p_{m,3} + 0.25\,p_{m,4}\right) \\ 0.1875\left(0.1875\,p_{m,3} + 0.25\,p_{m,4}\right) \\ 0.25 \times 0.0625\,p_{m,4}\end{array}\right\}.\end{aligned} \tag{9.6}$$

Thus in the case of two block interpretation model and M sets of weights $\{p\}_m$, we can accumulate $2M$ effective values and sets of the affecting factors (Table 9.1) permitting making up an excessive system for evaluating the four actual hydraulic resistivities g_1, g_2, g_3, g_4.

To solve the above excessive system, the least squares method can be applied. That is, the unknown values g_1, g_2, g_3, g_4 are considered as the regression coefficients minimizing sum

$$s_m = \sum_{m=1}^{2M}\left(g_1 w_{m,1} + g_2 w_{m,2} + g_3 w_{m,3} + g_4 w_{m,4} - \hat{g}_m\right)^2. \tag{9.7}$$

Table 9.1 Set consisting of M subsets of weights for evaluating the real-life hydraulic resistivities as regression coefficients

Eq. No.	Weights	Effective parameters	Affecting factors
1	$\{p\}_1$	$\hat{g}_{1,1}$	$\{w_{1,1,1}, w_{1,1,2}, w_{1,1,3}, w_{1,1,4}\}$
2		$\hat{g}_{1,2}$	$\{w_{1,2,1}, w_{1,2,2}, w_{1,2,3}, w_{1,2,4}\}$
3	$\{p\}_2$	$\hat{g}_{2,3}$	$\{w_{2,3,1}, w_{2,3,2}, w_{2,3,3}, w_{2,3,4}\}$
4		$\hat{g}_{2,4}$	$\{w_{2,4,1}, w_{2,4,2}, w_{2,4,3}, w_{2,4,4}\}$
...	...	...	...
$2m-1$	$\{p\}_m$	$\hat{g}_{m,2m-1}$	$\{w_{m,2m-1,1}, w_{m,2m-1,2}, w_{m,2m-1,3}, w_{m,2m-1,4}\}$
$2m$		$\hat{g}_{m,2m}$	$\{w_{m,2m,1}, w_{m,2m,2}, w_{m,2m,3}, w_{m,2m,4}\}$
...	...	...	...
$2M-1$	$\{p\}_M$	$\hat{g}_{M,2M-1}$	$\{w_{M,2M-1,1}, w_{M,2M-1,2}\ w_{M,2M-1,3}, w_{M,2M-1,4}\}$
$2M$		$\hat{g}_{M,2M}$	$\{w_{M,2M,1}, w_{M,2M,2}, w_{M,2M,3}, w_{M,2M,4}\}$

Applying the standard least squares technique to Sum 9.7 leads to the system of four equations:

$$\begin{aligned}
g_1\sum_{m=1}^{2M} w_{m,1}^2 + g_2\sum_{m=1}^{2M} w_{m,1}w_{m,2} + g_3\sum_{m=1}^{2M} w_{m,1}w_{m,3} + g_4\sum_{m=1}^{2M} w_{m,1}w_{m,4} &= \sum_{m=1}^{2M} w_{m,1}\hat{g}_{m,1}\\
g_1\sum_{m=1}^{2M} w_{m,2}w_{m,1} + g_2\sum_{m=1}^{2M} w_{m,2}^2 + g_3\sum_{m=1}^{2M} w_{m,2}w_{m,3} + g_4\sum_{m=1}^{2M} w_{m,2}w_{m,4} &= \sum_{m=1}^{2M} w_{m,2}\hat{g}_{m,2}\\
g_1\sum_{m=1}^{2M} w_{m,3}w_{m,1} + g_2\sum_{m=1}^{2M} w_{m,3}w_{m,2} + g_3\sum_{m=1}^{2M} w_{m,3}^2 + g_4\sum_{m=1}^{2M} w_{m,3}w_{m,4} &= \sum_{m=1}^{2M} w_{w,3}\hat{g}_{m,3}\\
g_1\sum_{m=1}^{2M} w_{m,4}w_{m,1} + g_2\sum_{m=1}^{2M} w_{m,4}w_{m,2} + g_3\sum_{m=1}^{2M} w_{m,4}w_{m,3} + g_4\sum_{m=1}^{2M} w_{m,4}^2 &= \sum_{m=1}^{2M} \hat{g}_{m,4}w_{m,4}.
\end{aligned} \tag{9.8}$$

Solving the above system yields value $g_{1:4}$.

Case 9.1.1 Let the available observations on the squared water table elevations be those obtained and used in Cases 6.2.2 and 6.2.1 (Tables 9.2 and 9.3). The squared elevations in Table 9.2 are obtained with the following distribution of hydraulic conductivities: $K_1 = 0.1$, $K_2 = 0.2$, $K_3 = 0.9$ and $K_4 = 1$ m/day in intervals (0, 25], (25, 50], (50, 75] and (75, 100] m correspondingly.

Applying the above procedure to the data presented in Table 9.2 with use of a hundred transforming mechanisms ($M = 50$) yields

$$K_1 = 0.1000, K_2 = 0.2000, K_3 = 0.9001, K_4 = 1.0000\,\mathrm{m/day}.$$

That is, the above procedure solved the inverse problem accurately.

Since the inverse problem is prone to incorrectness, it is interesting to watch how the errors in the initial data affect the results. Thus, rounding the squared water table elevations in Table 9.2 to three digits to the right from the decimal point results in solution:

$$K_1 = 0.1000,\ K_2 = 0.1999,\ K_3 = 0.9014,\ K_4 = 1.0081\,\mathrm{m/day}.$$

Rounding the same data to two decimal digits yields:

$$K_1 = 0.0999,\ K_2 = 0.2003,\ K_3 = 0.8929,\ K_4 = 1.0417\,\mathrm{m/day}.$$

Rounding the same data to one decimal digit brings:

Table 9.2 "Observed" data in Case 6.2.2

i	1	2	3	4
x (m)	25	50	75	100
h^2 (m^2)	4.3850	5.9475	6.1558	6.2183

$$K_1 = 0.1,\ K_2 = 0.2,\ K_3 = 0.6,\ K_4 = 1.49 \times 10^{13}\,\mathrm{m/day}.$$

The last result, at least in respect to K_4 is unacceptably corrupt. (The error in value K_3, about 30 %, could be considered as acceptable by many practitioners).

The last result demonstrates incorrectness, instability, of this inverse problem. The reason is that the slope of the water table approaches the water divide at $x = 100$ m and becomes about horizontal: the difference between water table elevations at $x_3 = 75$ m and $x_4 = 100$ m is less than 2 cm. The situation is close to that presented in Fig. 4.1. It is difficult to expect that under such circumstance there exists a mathematical manipulation able to convert the problem in a correct one. If it is impossible to improve the accuracy of the initial data, we have to exclude the data related to location x_4 from consideration and limit ourselves finding the hydraulic conductivities K_1, K_2 and K_3. For evaluating the hydraulic conductivity of the fourth body, the aquitard must be perturbed by a pumping test or in some other way.

The data on Case 6.2.2 have been selected because reproducing the thicknesses aquifer in this case is much worse than in Case 6.2.1. Nevertheless it is interesting to apply to the data of Case 6.2.1 the above procedure. The corresponding values of the conductivity in Case 6.2.2 are $K_1 = 1$, $K_2 = 0.9$, $K_3 = 0.2$, $K_4 = 0.1$ m/day. The squared thicknesses of the aquifer for this case are presented in Table 9.3.

Application of the above described procedure to the data in Table 9.2 yields the following results

$$K_1 = 1.0000,\ K_2 = 0.9001,\ K_3 = 0.2000,\ K_4 = 0.1000\,\mathrm{m/day}.$$

Rounding the squared water table elevations in Table 9.3 to three decimal digits to the right from the decimal point results in solution:

$$K_1 = 0.9989,\ K_2 = 0.9006,\ K_3 = 0.2001,\ K_4 = 0.1000\,\mathrm{m/day}.$$

Rounding the same data to two decimal digits yields:

$$K_1 = 0.9943,\ K_2 = 0.9191,\ K_3 = 0.1995,\ K_4 = 0.0992\,\mathrm{m/day}.$$

Rounding the same data to one decimal digit brings:

$$K_1 = 1.1218,\ K_2 = 0.7812,\ K_3 = 0.2083,\ K_4 = 0.0893\,\mathrm{m/day}.$$

These results seem to be more stable and accurate due, probably, the absence of the "observations" which are not undistinguishable practically.

Table 9.3 'Observed' data in Case 6.2.1

i	1	2	3	4
x (m)	25	50	75	100
h^2 (m^2)	0.4475	0.7947	1.7322	2.3572

Case 9.1.2 Let the interpretational model be the simplest one, i.e., homogeneous. For this model the relationship between the effective hydraulic resistivity and the effective squared water table can be presented as following

$$\begin{aligned}
\hat{h}_{m,1}^2 - h_0^2 &= 0.4375\,\hat{g}_m \\
\hat{h}_{m,2}^2 - h_0^2 &= 0.75\,\hat{g}_m \\
\hat{h}_{m,3}^2 - h_0^2 &= 0.9375\,\hat{g}_m \\
\hat{h}_{m,4}^2 - h_0^2 &= \hat{g}_m.
\end{aligned} \tag{9.9}$$

Criterion 9.2 takes form

$$\begin{aligned}
s_m = p_{m,1}\left(0.4375\,\hat{g}_m - \left(h_1^2 - h_0^2\right)\right)^2 + p_{m,2}\left(0.75\,\hat{g}_m - \left(h_2^2 - h_0^2\right)\right)^2 \\
+ p_{m,3}\left(0.9375\,\hat{g}_m - \left(h_3^2 - h_0^2\right)\right)^2 + p_{m,4}\left(\hat{g}_m - \left(h_4^2 - h_0^2\right)\right)^2
\end{aligned} \tag{9.10}$$

where $\{p\}_m$ is the mth set of weights. Applying the standard least square technique yields

$$\hat{g}_m = \frac{0.4375\,p_{p,1}\left(h_1^2 - h_0^2\right) + 0.75\,p_{m,2}\left(h_2^2 - h_0^2\right) + 0.9375\,p_{m,3}\left(h_3^2 - h_0^2\right) + p_{m,4}\left(h_4^2 - h_0\right)}{0.4375^2\,p_{m,1} + 0.75^2\,p_{m,2} + 0.9375^2\,p_{m,3} + p_{m,4}}. \tag{9.11}$$

The actual squared water table elevations are described by the expressions

$$\begin{aligned}
h_1^2 - h_0^2 &= 0.4375 g_1 \\
h_2^2 - h_0^2 &= 0.4375 g_1 + 0.3125 g_2 \\
h_3^2 - h_0^2 &= 0.4375 g_1 + 0.3125 g_2 + 0.1875 g_3 \\
h_4^2 - h_0^2 &= 0.4375 g_1 + 0.3125 g_2 + 0.1875 g_3 + 0.0625 g_4.
\end{aligned} \tag{9.12}$$

Substituting Expressions 9.12 in Eq. 9.11 and combining the terms containing the same real world hydraulic resistivities yield the following affecting factors

$$\begin{aligned}
w_{m,1} &= 0.4375\left(0.4375\,p_{m,1} + 0.75\,p_{m,2} + 0.9375\,p_{m,3} + p_{m,4}\right)/c_m \\
w_{m,2} &= 0.3125\left(0.75\,p_{m,2} + 0.9375\,p_{m,3} + p_{m,4}\right)/c_m \\
w_{m,3} &= 0.1875\left(0.9375\,p_{m,3} + p_{m,4}\right)/c_m \\
w_{m,4} &= 0.0625\,p_{m,4}/c_m
\end{aligned} \tag{9.13}$$

where

$$c_m = 0.4375^2\,p_{m,1} + 0.75^2\,p_{m,2} + 0.9375^2\,p_{m,3} + p_{m,4}. \tag{9.14}$$

Thus, we obtain Regression 9.1

$$g_1 w_{m,1} + g_2 w_{m,2} + g_3 w_{m,3} + g_4 w_{m,4} = \hat{g}_m \tag{9.15}$$

and find the pertinent hydraulic resistivities as coefficients of the above regression in which affecting $w_{m,i}$ factors play part of the independent variables and $\hat{g}_m$ is calculated based on the observations.

The homogeneous model yields results which are exactly the same as in Case 9.1.1, though the model and the inverse problem solving are considerably simpler.

Case 9.1.3 Cases 9.1.1–9.1.2 demonstrated that the transforming mechanisms can be successfully applied for inverse problem solving in some situations. But it is not always so. Let us assume now that in the inverse problem considered above the geological object consists of eight geological bodies with the boundaries at locations $X_0 = 0$, $X_1 = 12.5$, $X_2 = 25$, $X_3 = 37.5$, $X_4 = 50$, $X_5 = 62.5$, $X_6 = 75$, $X_7 = 87.5$ and $X_8 = 100$ m with the constant hydraulic conductivities within intervals $[X_{j-1}, X_j]$: K_1, K_2, K_3, K_4, K_5, K_6, K_7 and K_8 (hydraulic resistivities $g_1 = 1/K_1$, $g_2 = 1/K_2$, $g_3 = 1/K_3$, $g_4 = 1/K_4$, $g_5 = 1/K_5$, $g_6 = 1/K_6$, $g_7 = 1/K_7$ and $g_8 = 1/K_8$). The monitoring network and the observed squared water table elevations are those presented in Table 9.2. The recharge rate also remains the same, $N = 0.0001$ m/day. The task is to find the hydraulic conductivities K_1, K_2, K_3, K_4, K_5, K_6, K_7, and K_8 based on the available water table elevations using a homogeneous interpretation model.

The approach to solving this inverse problem remains the same as in the previous cases. Namely, the unknown hydraulic resistivities g_1 to g_8 are coefficients of the linear regression

$$g_1 w_{m,1} + g_2 w_{m,2} + g_3 w_{m,3} + g_4 w_{m,4} + g_5 w_{m,5} + g_6 w_{m,6} + g_7 w_{m,7} + g_8 w_{m,8} = \hat{g}_m \tag{9.16}$$

where $w_{m,i}$ ($i = 1$–8) are the pertinent affecting factors corresponding to the set of weights $\{p\}_m = \{p_{m,1}, p_{m,2}, p_{m,3}, p_{m,4}\}$ and playing independent variables, $\hat{g}_m$ is the known pertinent effective value of the hydraulic resistivity, 'the observation'. Thus the goal is to make up large number of sets of the affecting factors $\{w\}_{m,} = \{w_{m,1}, w_{m,2},\ldots, w_{m,8}\}$ and the pertinent effective parameters $\hat{g}_m$.

The effective resistivity $\hat{g}_m$ corresponding to the set of weights $\{p\}_m = \{p_{m,1}, p_{m,2}, p_{m,3}, p_{m,4}\}$ can be calculated by Eq. 9.9. In the case of the eight-body real world, Eq. 9.9 become

$$\begin{aligned}
h_1^2 - h_0^2 &= 0.2344 g_1 + 0.2031 g_2 \\
h_2^2 - h_0^2 &= 0.2344 g_1 + 0.2031 g_2 + 0.1791 g_3 + 0.1406 g_4 \\
h_3^2 - h_0^2 &= 0.2344 g_1 + 0.2031 g_2 + 0.1791 g_3 + 0.1406 g_4 + 0.1094 g_5 + 0.0781 g_6 \\
h_4^2 - h_0^2 &= 0.2344 g_1 + 0.2031 g_2 + 0.1791 g_3 + 0.1406 g_4 + 0.1094 g_5 + 0.0781 g_6 \\
&\quad + 0.0469 g_7 + 0.01563 g_8.
\end{aligned} \tag{9.17}$$

Substituting Expressions 9.17 in Eq. 9.11 and calculating multipliers in terms with different $g_{1:8}$ yield the following affecting factors

$$
\begin{aligned}
w_{m,1} &= \frac{0.2344\left(0.4375p_{m,1} + 0.75p_{m,2} + 0.9375p_{m,3} + p_{m,4}\right)}{c_m}; & w_{m,2} &= \frac{0.2031w_{m,1}}{0.2344} \\
w_{m,3} &= \frac{0.1719\left(0.75p_{m,2} + 0.9375p_{m,3} + p_{m,4}\right)}{c_m}; & w_{m,4} &= \frac{0.1406w_{m,3}}{0.1719} \\
w_{m,5} &= \frac{0.1094\left(0.9375p_{m,3} + p_{m,4}\right)}{c_m}; & w_{m,6} &= \frac{0.0781w_{m,4}}{0.1094} \\
w_{m,7} &= \frac{0.0469p_{m,4}}{c_m}; & w_{m,8} &= \frac{0.01563p_{m,4}}{0.0469}
\end{aligned}
\tag{9.18}
$$

where the denominator c_m is defined by Eq. 9.14.

Now we can apply standard least squares technique for evaluating the unknown hydraulic resistivities $g_{1:8}$, the regression coefficients of Regression 9.16. Based on the data presented in Table 9.2 and $M = 100$ corresponding to 100 sets of independent variables $\{w\}_m$ and the known values $\hat{g}_m$ we obtain

$$K = [-0.0321, 0.0262, -0.0596, 0.0435, 0.0848, -0.2215, -0.0021, 0.0007]\,\mathrm{m/day}$$

instead of the factual hydraulic conductivities:

$$K = [0.1, 0.1, 0.2, 0.2, 0.9, 0.9, 1, 1]\,\mathrm{m/day}.$$

Thus, the inverse problem formulation in Case 9.1.3 is incorrect. The mathematical cause of the incorrectness is bad conditioning of the system for finding the hydraulic resistivities $g_{1:8}$. It happened because the affecting factors are mutually dependant and not enough diverse. (This is not the case for evaluating the affecting factors per se by the two-level modeling. Indeed, we are free to select any values of the real world parameters and to make them as diverse as we want). However, the main reason is mismatch of the complexity of the object and the data for solving the inverse problem. What may provide comfort is the possibility to establish correctness or incorrectness of formulation of an inverse problem before starting field explorations by the-two-level modeling and to look for the appropriate changing of the methodology of the investigations.

9.2 Borden Landfill: Evaluating Actual Recharge Rates

Let the simulation model in Sect. 4.4 represent the real geological object. The goal is to evaluate the actual recharge rates pertaining to intervals (300, 600], (600, 800] and (800, 900] m assigned by Frind and Hokkanen (1987). The data for solving the inverse problems are presented in Table 9.4 (cf. Tables 6.11 and 6.12). They comprise the available observations on the water table and the streamline starting at $x = 300$ m and the expressions for calculating the total flux at the points of the

Table 9.4 Data for solving inverse problems for the Borden landfill

#	x	H	$v = H - Y$	Y	H_S	$u = H_S - Y$	Q
0	300	222.31	17.99	204.31	222.31	17.99	Q_s
1	400	222.23	16.06	206.17	219.25	13.08	$Q_s + 100N_3$
2	500	222.11	12.56	209.55	218.26	8.71	$Q_s + 200N_3$
3	600	221.95	11.09	210.85	217.46	6.61	$Q_s + 300N_3$
4	700	221.72	10.39	211.33	216.07	4.74	$Q_s + 300N_3 + 100N_4$
5	800	221.42	9.56	211.86	215.47	3.61	$Q_s + 300N_3 + 200N_4$
6	900	221.04	8.24	212.79	215.67	2.88	$Q_s + 300N_3 + 200N_4 + 100N_5$

observations. (The recharge rates in interval [0, 300] m and the total flux $Q_S = Q(300) = 0.1253$ m^2/day are assumed known.)

Case 9.2.1 Let the interpretation model be a homogeneous with respect to recharge pattern for $x > 300$ m (Fig. 9.1). The approach to solving this inverse problem is about the same as in the previous section. Namely, the goal is to make up a manifold of transforming mechanisms by applying different subsets of weights to the observed data, $u_{1:6}$. As soon as the manifold is obtained, the corresponding transforming mechanisms are considered as linear regressions with the unknown regression coefficients $N_{3:5}$. The effective

$$N_3 w_{m,1} + N_4 w_{m,2} + N_5 w_{m,3} = \hat{N}_m \tag{9.19}$$

recharge rates $\hat{N}_m$, corresponding to the random set of weights $\{p_{m,1:6}\}$, can be evaluated based on the available observations. With all necessary data accumulated, the unknown recharge rates $N_{3:5}$ can be obtained by standard least squares technique as solution of the following system

$$\begin{aligned}
N_3 \sum_{m=1}^{M} w_{m,1}^2 + N_4 \sum_{m=1}^{M} w_{m,1} w_{m,2} + N_5 \sum_{m=1}^{M} w_{m,1} w_{m,3} &= \sum_{m=1}^{M} w_{m,1} \hat{N}_m \\
N_3 \sum_{m=1}^{M} w_{m,2} w_{m,1} + N_4 \sum_{m=1}^{M} w_{m,2}^2 + N_5 \sum_{m=1}^{M} w_{m,2} w_{m,3} &= \sum_{m=1}^{M} w_{m,2} \hat{N}_m \\
N_3 \sum_{m=1}^{M} w_{m,3} w_{m,1} + N_4 \sum_{m=1}^{M} w_{m,3} w_{m,2} + N_5 \sum_{m=1}^{M} w_{m,3}^2 &= \sum_{m=1}^{M} w_{m,3} \hat{N}_m.
\end{aligned} \tag{9.20}$$

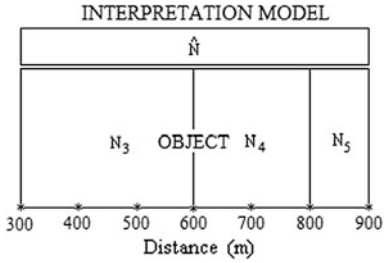

Fig. 9.1 Case 9.2.1: homogeneous interpretational model for evaluating recharge rates N_3, N_4 and N_5

In Sect. 6.4, the transforming mechanism has been obtained analytically for uniform weighting. The same can be done for non-uniform weighting. Let us assume that recharges N_3, N_4 and N_5 are known. The effective recharge rates corresponding to weighting $\{p_{m,1:6}\}$ and the above recharge pattern can be obtained straightforwardly, minimizing criterion

$$s_m = \sum_{i=1}^{6} p_{m,i}\left(\hat{Q}_{m,i} - Q_i\right)^2 u_i^2 \tag{9.21}$$

where Q_i and $\hat{Q}_{m,i}$ are the actual and effective total fluxes at the observation points, presented in Table 9.5. The standard least squares procedure requires solving for equation

$$\sum_{i=1}^{6} p_{m,i} u_i^2 \left(\hat{Q}_{m,i} - Q_i\right) \frac{d\hat{Q}_{m,i}}{d\hat{N}_m} = 0. \tag{9.22}$$

Substituting in Eq. 9.22 the expressions for Q_i and $\hat{Q}_{m,i}$ from Table 9.5 and solving it for $\hat{N}_m$ yield Eq. 9.19 in which

$$w_{m,1} = b_{m,1}/c_m, \quad w_{m,2} = b_{m,2}/c_m, \quad w_{m,3} = b_{m,3}/c_m \tag{9.23}$$

and

$$\begin{aligned} c_m &= p_{m,1}u_1^2 + 4\,p_{m,2}u_2^2 + 9\,p_{m,3}u_3^2 + 16\,p_{m,4}u_4^2 + 25\,p_{m,5}u_5^2 + 36\,p_{m,6}u_6^2 \\ b_{m,1} &= p_{m,1}u_1^2 + 4\,p_{m,2}u_2^2 + 9\,p_{m,3}u_3^2 + 12\,p_{m,4}u_4^2 + 15\,p_{m,5}u_5^2 + 18\,p_{m,6}u_6^2 \\ b_{m,2} &= 4\,p_{m,4}u_4^2 + 10\,p_{m,5}u_5^2 + 12\,p_{m,6}u_6^2 \\ b_{m,3} &= 6\,p_{m,6}u_6^2. \end{aligned} \tag{9.24}$$

(It is easy to check that, as expected, the affecting factors in Mechanisms 9.23 sum to one).

Thus, the affecting factors comprising coefficients of System 9.20 are obtained. To complete creating System 9.20, it is necessary to obtain the right-hand terms including $\hat{N}_m$, the actual effective recharge rate corresponding to each set of weights $\{p_{m,\ 1:6}\}$. $\hat{N}_m$ can be found by minimization of criterion

Table 9.5 Case 9.2.1: expressions for calculating total fluxes Q_i and $\hat{Q}_{m,i}$

#	x	Q	$\hat{Q}_m$
0	300	Q_S	Q_S
1	400	$Q_S + 100N_3$	$Q_S + 100\hat{N}_m$
2	500	$Q_S + 200N_3$	$Q_S + 200\hat{N}_m$
3	600	$Q_S + 300N_3$	$Q_S + 300\hat{N}_m$
4	700	$Q_S + 300N_3 + 100N_4$	$Q_S + 400\hat{N}_m$
5	800	$Q_S + 300N_3 + 200N_4$	$Q_S + 500\hat{N}_m$
6	900	$Q_S + 300N_3 + 200N_4 + 100N_5$	$Q_S + 600\hat{N}_m$

$$s_m = \sum_{i=1}^{6} p_{m,i}\left(\hat{Q}_{m,i}u_i - Q_S v_i\right)^2 \tag{9.25}$$

(cf. criterion 6.39) leading to the equation

$$\begin{aligned} &100\left(p_{m,1}u_1^2 + 4\,p_{m,2}u_2^2 + 9\,p_{m,3}u_3^2 + 16\,p_{m,4}u_4^2 + 25\,p_{m,5}u_5^2 + p_{m,6}u_6^2\right)\hat{N}_m \\ &= Q_S\begin{pmatrix} p_{m,1}u_1(v_1 - u_1) + 2\,p_{m,2}u_2(v_2 - u_2) + 3\,p_{m,3}u_3(v_3 - u_3) + \\ 4\,p_{m,4}u_4(v_4 - u_4) + 5\,p_{m,5}u_5(v_5 - u_5) + 6\,p_{m,6}u_6(v_6 - u_6) \end{pmatrix}. \end{aligned} \tag{9.26}$$

Substituting the data from Tables 9.4 and 9.5 in Eq. 9.26 yields

$$\hat{N}_m = \frac{Q_S}{100}\frac{\sum_{i=1}^{6} p_{m,i}iu_i(v_i - u_i)}{\sum_{i=1}^{6} p_{m,i}i^2u_i^2}, \quad (Q_S = 0.1253\,\mathrm{m}^2/\mathrm{day}). \tag{9.27}$$

Now System 9.20 can be made up and solved. The results of several realizations of the above procedure are presented in Table 9.6. They seem consistent. The results obtained for $M = 50$ are presented in Fig. 9.2. They are practically satisfying the travel time to x equal 900 and 950 m is about 38.9 and 40 years. The magnitude of the maximal error in reproducing the stream line is at $x = 500$ m. It is less than 5 cm which is better than that obtained in process of the model identification (Sect. 4.4). However for $x > 800$ m the error grows considerably, meaning that the recharge rate N_5 needs correction. Besides, the condition numbers of Systems 9.20 for different M are large.

Fortunately the interpretation model permits manual correcting. Indeed, the model is such that the recharge rate N_5 for $x > 800$ m does not affect the previous observations. Thus the recharge pattern

$$N_3 = 10.29,\ N_4 = 22.75 \quad \text{and} \quad N_5 = 8\,\mathrm{cm/year}$$

makes magnitude of the error at $x = 900$ m close to 2 cm. (Compare to $N_3 = 10.2$, $N_4 = 23$ and $N_5 = 8.36$ cm/year, Table 4.4, The travel time to x equal 900 and 950 m are about 39 and 40.2 years).

Case 9.2.2 Let us change the interpretation model. Now it comprises two blocks: interval (300, 600] m constitutes the first homogeneous block with the effective

Table 9.6 Some results of solving inverse problem in Case 9.2.1 (M is the number of simulations)

M	Recharge rates (cm/year)			Condition number System 9.20
	N_3	N_4	N_5	
10	10.38	22.53	16.70	6,017
50	10.29	22.75	18.33	4,261
250	10.31	22.68	18.89	3,992
1,250	10.30	22.68	18.59	4,247
6,250	10.30	22.66	18.66	3,897

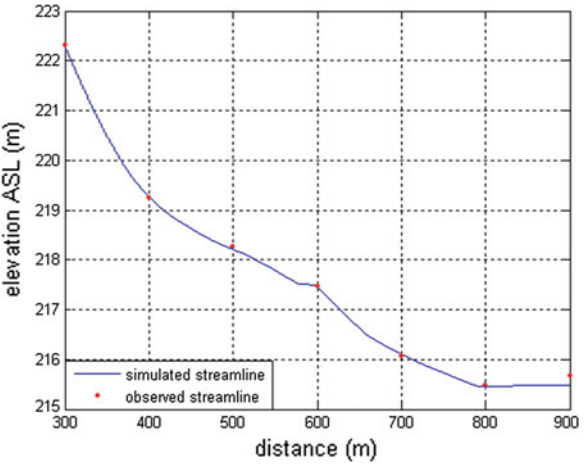

Fig. 9.2 Case 9.2.1: reproducing the streamline starting at $x = 300$ m by the recharge rates yielded by inverse problem solving

recharge rate $\hat{N}_1$; interval (600, 900] m constitutes the second one with the recharge rate $\hat{N}_2$ (Fig. 9.3).

In general the procedure of solving the inverse problem in this case does not differ from the previous one. The goal is to create and solve the system of equations like System 9.20, The available information remains the same (Table 9.4). Since two effective recharge rates exist: $\hat{N}_{m,1}$ for the first model block and $\hat{N}_{m,2}$ for two different mechanism should be involved.

$$\begin{aligned} \hat{N}_{m,1} &= w_{m,1,1}N_3 + w_{m,1,2}N_4 + w_{m,1,3}N_5 \\ \hat{N}_{m,2} &= w_{m,2,1}N_3 + w_{m,2,2}N_4 + w_{m,2,3}N_5. \end{aligned} \tag{9.28}$$

The necessity to work with two transforming mechanisms could complicate the problems in general, but not in this case. According to Properties 1 and 2 of the transforming mechanisms, Sect. 5.3, the affecting factors $w_{m,1,1} = 1$, $w_{m,1,2} = -w_{m,1,3}$, $w_{m,2,1} = 0$, $w_{m,2,3} = 1 - w_{m,2,2}$ and Mechanisms 9.28 can be rewritten as

$$\begin{aligned} \hat{N}_{m,1} &= N_3 + w_{m,1,2}N_4 - w_{m,1,2}N_5 \\ \hat{N}_{m,2} &= w_{m,2,2}N_4 + \left(1 - w_{m,2,2}\right)N_5. \end{aligned} \tag{9.29}$$

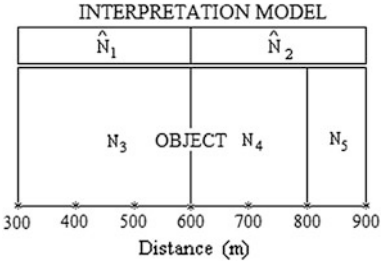

Fig. 9.3 Case 9.2.2: two-block interpretation model for finding recharge rates N_3, N_4 and N_5

However we will consider all affecting factors as unknown and will use their properties to control the calculations.

Mechanisms 9.28 can be evaluated analytically as it has been done in Case 9.2.1, though it may be a cumbersome task. We come back to the standardized procedure described in Sects. 8.1–8.3. Let us assign R sets of the recharge rates $\{N_{r,3}, N_{r,4}, N_{r,5}\}$ at random. Then for a given set of weights $\{p_{m,1:6}\}$ and each sets $\{N_{r,3:5}\}$, the effective recharge rates $\hat{N}_{m,r,1}$ and $\hat{N}_{m,r,2}$ are evaluated by minimization of criterion

$$s_{m,r} = \sum_{i=1}^{6} p_{m,i} u_i^2 \left(\hat{Q}_{m,r,i} - Q_{r,i}\right)^2 \tag{9.30}$$

(cf. criterion 9.26) where u_i is the observed thickness of the aquifer's part below the streamline S. Expressions for calculating the effective total fluxes $\hat{Q}_{m,r,1}$ are presented in Table 9.7. The standard least squares method leads to system of two equations

$$\sum_{i=1}^{6} p_{m,i} u_i^2 \left(\hat{Q}_{m,r,i} - Q_{r,i}\right) \frac{d\hat{Q}_{m,r,i}}{d\hat{N}_{m,r,j}} = 0, \quad j = 1, 2 \tag{9.31}$$

which can be presented explicitly as

$$\begin{aligned}
&\left(\sum_{i=1}^{3} i^2 p_{m,i} u_i^2 + 9\sum_{i=4}^{6} p_{m,i} u_i^2\right)\hat{N}_{m,r,1} + 3\left(\sum_{i=4}^{6} (i-3) p_{m,i} u_i^2\right)\hat{N}_{m,r,2} \\
&= \left(\sum_{i=1}^{2} i^2 p_{m,i} u_i^2 + 9\sum_{i=3}^{6} p_{m,i} u_i^2\right)N_{r,3} + 3\left(\sum_{i=4}^{6} (i-3) p_{m,i} u_i^2 - p_{m,6} u_i^2\right)N_{r,4} \\
&\quad + 3\, p_{m,6} u_6^2 N_{r,5} \\
&3\left(\sum_{i=4}^{6} (i-3) p_{m,i} u_i^2\right)\hat{N}_{m,r,1} + \left(\sum_{i=4}^{6} (i-3)^2 p_{m,i} u_i^2\right)\hat{N}_{m,r,2} = 3\left(\sum_{i=4}^{6} (i-3) p_{m,i} u_i^2\right)N_{r,3} \\
&\quad + \left(p_{m,4} u_4^2 + 4\, p_{m,5} u_5^2 + 6\, p_{m,6} u_6^2\right)N_{r,4} + 3\, p_{m,6} u_6^2 N_{r,5}.
\end{aligned} \tag{9.32}$$

Table 9.7 Case 9.2.2: expressions for calculating total fluxes $Q_{r,i}$ and $\hat{Q}_{m,r,i}$

#	x	Q_r	$\hat{Q}_{m,r}$
0	300	Q_S	Q_S
1	400	$Q_S + 100N_{r,3}$	$Q_S + 100\hat{N}_{m,r,1}$
2	500	$Q_S + 200N_{r,3}$	$Q_S + 200\hat{N}_{m,r,1}$
3	600	$Q_S + 300N_{r,3}$	$Q_S + 300\hat{N}_{m,r,1}$
4	700	$Q_S + 300N_{r,3} + 100N_{r,4}$	$Q_S + 300\hat{N}_{m,r,1} + 100\hat{N}_{m,r,2}$
5	800	$Q_S + 300N_{r,3} + 200N_{r,4}$	$Q_S + 300\hat{N}_{m,r,1} + 200\hat{N}_{m,r,2}$
6	900	$Q_S + 300N_{r,3} + 200N_{r,4} + 100N_{r,4}$	$Q_S + 300\hat{N}_{m,r,1} + 300\hat{N}_{m,r,2}$

Solving System 9.32 yields M coupled values of the effective recharge rates $\hat{N}_{m,r,1}$ and $\hat{N}_{m,r,2}$. Substituted values $\hat{N}_{m,r,1}$ and $\hat{N}_{m,r,2}$ in Eq. 9.28 which for a fixed m and different r can be rewritten as

$$\begin{aligned} w_{m,1,1}N_{r,3} + w_{m,1,2}N_{r,4} + w_{m,1,3}N_{r,5} &= \hat{N}_{m,r,1} \\ w_{m,2,1}N_{r,3} + w_{m,2,2}N_{r,4} + w_{m,2,3}N_{r,5} &= \hat{N}_{m,r,2} \end{aligned} \tag{9.33}$$

we obtain the excessive system of linear equations for evaluating the unknown affecting factors $w_{m,j,1:3}$ $(j = 1, 2)$ which could be solved by the least squares method.

The next step is evaluating actual effective values $\hat{N}_{m,1}$ and $\hat{N}_{m,2}$ corresponding to different sets of weights applying the data from Tables 9.4 and 9.7 by minimization of Criterion 9.25

$$\begin{aligned} &\left(p_{m,1}u_1^2 + 4p_{m,2}u_2^2 + 9\sum_{i=3}^{6} p_{m,i}u_i^2\right)\hat{N}_{m,1} + 3\sum_{i=4}^{6} p_{m,i}(i-3)u_i^2\hat{N}_{m,2} \\ &= \frac{Q_S}{100}\left(p_{m,1}u_1(v_1 - u_1) + 2p_{m,2}u_2(v_2 - u_2) + 3\sum_{i=3}^{6} p_{m,i}u_i(v_i - u_i)\right) \\ &3\left(\sum_{i=4}^{6}(i-3)p_{m,i}u_i^2\right)\hat{N}_1 + \left(\sum_{i=4}^{6}(i-3)^2 p_{m,i}u_i^2\right)\hat{N}_2 = \frac{Q_S}{100}\left(\sum_{i=4}^{6}(i-3)p_{m,i}u_i(v_i - u_i)\right). \end{aligned} \tag{9.34}$$

Its solution is $2M$ values of effective recharge rates $\hat{N}_{m,1}$ and $\hat{N}_{m,2}$.

Now the system of equations similar to System 9.20 can be made up and solved. Several results of realization of the above procedure are presented in Table 9.8. They are close to those obtained in Case 9.2.1. Note that condition numbers of System 9.20 in Case 9.2.2 is much better than in Case 9.2.1, meaning that the inverse problem in Case 9.2.2 is practically stable.

Case 9.2.3 Let the interpretation model be an exact copy of the real object. This means that now for $x > 300$ m it comprises three blocks in intervals (300, 600], (600, 800], $x > 800$ m. In this case the above approach, that is, creating and solving systems of equations like System 9.19 does not work. Indeed, the three

Table 9.8 Some results of solving inverse problem in Case 9.2.2 (M is the number of simulations)

M	Recharge rates (cm/year)			Condition number
	N_3	N_4	N_5	
10	10.34	22.48	19.69	343
50	10.34	22.44	18.93	132
250	10.31	22.59	18.85	151
1,250	10.32	22.64	18.98	139
6,250	10.31	22.60	18.93	134

corresponding transforming mechanisms do not depend on weighting the observations and affecting factors stay the same: $w_{1,1} = w_{2,2} = w_{3,3} = 1$ and $w_{1,2} = w_{1,3} = w_{2,1} = w_{2,3} = w_{3,1} = w_{3,2} = 0$ for any weighting. This converts the current inverse problem into an optimization one: three unknown recharge rates N_3, N_4 and N_5 can be evaluated as the effective ones by straightforward application of the least squares method, that is, by minimization of criterion

$$s = \sum_{i=1}^{6} (Q_i u_i - Q_S v_i)^2 \tag{9.35}$$

where the total flux Q_i is defined by column $Q_{r,i}$ in Table 9.6 in which index 'r' is ignored. The standard least squares technique leads to the following system of linear equations:

$$\sum_{i=1}^{6} (Q_i u_i - Q_S v_i) u_i \frac{dQ_i}{dN_j} = 0, \quad j = 1, 2, 3 \tag{9.36}$$

which can be presented explicitly as

$$\begin{aligned}
&\left(\sum_{i=1}^{3} i^2 u_i^2 + 9\sum_{i=4}^{6} u_i^2\right) N_3 + 3\left(u_4^2 + 2u_5^2 + 2u_6^2\right) N_4 + 3u_6^2 N_5 \\
&= \frac{Q_S}{100}\left(u_1(v_1 - u_1) + 2u_2(v_2 - u_2) + 3\sum_{i=3}^{6} u_i(v_i - u_i)\right) \\
&3\left(u_4^2 + 2u_5^2 + 2u_6^2\right) N_3 + \left(u_4^2 + 4u_5^2 + 4u_6^2\right) N_4 + 2u_6^2 N_5 \\
&= \frac{Q_S}{100}\left(u_4(v_4 - u_4) + 2u_5(v_5 - u_5) + 2u_6(v_6 - u_6)\right) \\
&3u_6^2 N_3 + 2u_6^2 N_4 + u_6^2 N_5 = \frac{Q_S}{100} u_6(v_6 - u_6).
\end{aligned} \tag{9.37}$$

The results of solving System 9.37 are presented in Table 9.9. They are close to the results obtained in Cases 9.2.1 and 9.2.2.

Overestimation of rate N_5 obtained by solving the previous inverse problems with respect to the effective value $\hat{N}_5$ may cause some discomfort, though the difference between them can be considered as acceptable practically. The reason for the difference is expectable: too many assumptions and the assumptions about the structure of the real object and the steady-state water table specially. However,

Table 9.9 Results of solving inverse problem in Case 9.2.3

Recharge rates (cm/year)			Condition number
N_3	N_4	N_5	
10.31	22.64	18.98	254

different formulations of the considered inverse problem led to consistent results. This could be a good reason to reconsider the assumptions applied in the model identification.

9.3 Non-Linear Transforming Mechanisms: Illustrative Example

In principle solving inverse problems involving non-linear transforming mechanisms does not differs much from solving inverse problems involving linear ones. To make up closed or redundant systems of the equation resolving the problems, we may use weighting of the pertinent observations. Unfortunately, the obtained systems consist of equations like Eq. 7.20 and their solving may present a difficult mathematical problem. This issue can be avoided if to approach to the solving hydrogeological problem as they do in geophysics and, in particular, in the case of vertical electric sounding, using, the, so called, master curves for interpretation of the obtained data. This geophysical approach is discussed below. However, first we discuss some simple approximate ways of evaluation of actual parameters based on the transforming mechanisms presented in Sect. 7.2.

Let us come back to the object presented in Sect. 4.3, that is, to the confined aquifer comprising two homogeneous bodies having the hydraulic transmissivity T_1 and T_2 (Fig. 9.4). In the initial state the aquifer has the uniform distributions of the hydraulic heads $h(x,\ 0) = H_0$. At instant $t = 0$, the hydraulic head at $x = 2L = 100$ m jumps instantly to $h(2L,\ 0) = H_{2L}$ and stays the same: $h(2L,\ t) = H_{2L}$. At $x = 0$ the hydraulic head does not change: $h(0,\ t) = H_0$. (Without loosing generality, values H_0 and H_{2L} are assigned equal to 0 and 1 m.) The jump of the hydraulic head at $x = 2L$ initiates the process of changing the aquifer hydraulic heads. The goal is to evaluate the hydraulic conductivities, observing changing the hydraulic head $h(L,\ t)$ at $x = L = 50$ m and using homogeneous, one-block, interpretational model.

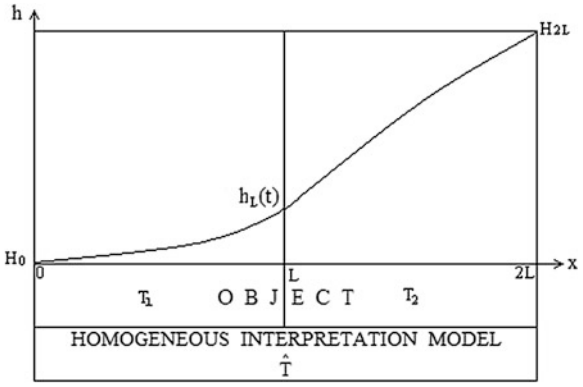

Fig. 9.4 Two body object and homogeneous interpretation model (confined aquifer with *horizontal* base)

The real observations can have an arbitrary time increment. For example, the observations can be conducted once a day, once a week, once in two weeks, and even be irregular. Therefore, the affecting factors in the corresponding inverse problems must be obtained by the implicit method (Sect. 7.3). However, the hydraulic heads often change slow in time. In such cases the transforming mechanism obtained in Sect. 7.2 by the explicit method may be an acceptable approximation of the transforming mechanism of the mechanism obtained in Sect. 7.3 even if the time increments are not very small. This mechanism, described by Eq. 7.14, is presented here for convenience:

$$\hat{T}_{i-1,i} = -\frac{h_{i-1}}{1-2h_{i-1}}T_1 + \frac{1-h_{i-1}}{1-2h_{i-1}}T_2, \tag{9.38}$$

where $h_{i\text{-}1} = h\,(L, t_{i-1})$, can be a satisfactory accurate approximation of Eq. 7.20. Equation 9.38 can be rewritten as

$$\hat{T}_{i-1,i} = T_1 w_{1,i} + T_2 w_{2,i} \tag{9.39}$$

where

$$w_{1,i} = -\frac{h_{i-1}}{1-2h_{i-1}} \quad \text{and} \quad w_{2,i} = \frac{1-h_{i-1}}{1-2h_{i-1}}. \tag{9.40}$$

The simplest way of solving the inverse problem is to consider Eq. 9.39 for two different instants t_i and t_j and solve the system of these two equations. Equation 9.39 can be interpreted also as a linear regression with T_1 and T_2 unknown actual transmissivities playing the part of regression coefficients and the affecting factors being the independent variable. (Note that $w_{1,i} = 1 - w_{2,i}$.) Then T_1 and T_2 can be found by the least squares method exactly in the same way as it has been done in the above cases with the linear transforming mechanisms. Several results of solving inverse problems based on Eq. 9.39 are presented in Table 9.10. The corresponding forward problems, providing "observations", are produced explicitly with the time increment $\Delta t = 0.1$ day (Sect. 7.2). According to the mechanism presented by Eq. 9.38 at the initial instant $t_0 = 0$ $h_{1,0} = 0$ also. Therefore, $\hat{T}_{i-1,i} = T_2$. If the observations are continued long enough and $h(t)$ becomes close to its asymptote, it follows from Eq. 4.31 that

Table 9.10 Solving inverse problems by Eq. 9.39

Actual transmissivity m^2/day		Interval between measurements (days)		
		1	7	14
T_1	T_2	Results of solving inverse problems: T_1, T_2 m^2/day		
0.1	0.9	0.1050, 0.9013	0.1050, 0.9013	0.1056, 0.9016
0.5	0.9	0.5005, 0.8999	0.5005, 0.8999	0.5006, 0.8999
0.9	0.9	0.9000, 0.9000	0.9000, 0.9000	0.9000, 0.9000
0.9	0.5	0.9000, 0.5001	0.9000, 0.5001	0.9000, 0.5001
0.9	0.1	0.9003, 0.1000	0.9003, 0.1000	0.9003, 0.1000

$$T_1 = \frac{1 - H_L}{H_L} T_2 \tag{9.41}$$

and so on.

There are many such ad hoc ways of solving inverse problems. Systematic approach to solving inverse problems, interpretation of observations, can be borrowed from geophysics. They work with effective parameters directly. Geophysicists call those parameters apparent and calculated, using usually homogeneous interpretational models. Since geological objects are not homogeneous, the apparent parameters vary with changing conditions under which they were obtained. Their changes are interpreted to evaluate the structures and properties of geological object by comparing the observed apparent parameters with the master curves calculated for geological objects of different structures and properties.

In this section, we also use a homogeneous interpretation model and our effective transmissivities are exactly what is called the apparent parameters in geophysics. The master curves presented in Figs. 9.5 and 9.6 correspond exactly to formulation of the forward and inverse problems discussed in this section: the object consists of two bodies with actual transmissivities T_1 and T_2, the effective transmissivity versus time are calculated for once a week observations at $x = L$. The curves factually depend on ratios T_1/T_2. The curves obtained based on actual observations is compared with the master curves. The master curve fitting the observations best provides the transmissivity T_1. (Transmissivity T_2 can be evaluated as the left asymptote of the curves.) The period of the observations is chosen as 182 days to avoid the instant of possible discontinuity of the transforming mechanisms when $T_1 < T_2$ as discussed in Case 7.2.2.

By the way the use of the geophysical master curves of electrical sounding, with three and four current electrodes and dipoles for interpreting data of pumping and injecting tests in not fully penetrating wells in steady-state regime was suggested by Gorokhovski and Jazvin (1970). At that time pumping tests lasting from several

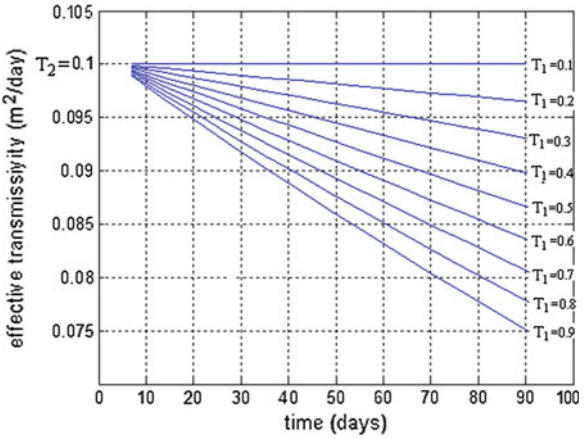

Fig. 9.5 Master *curves* for effective transmissivities for $T_2 < T_1$

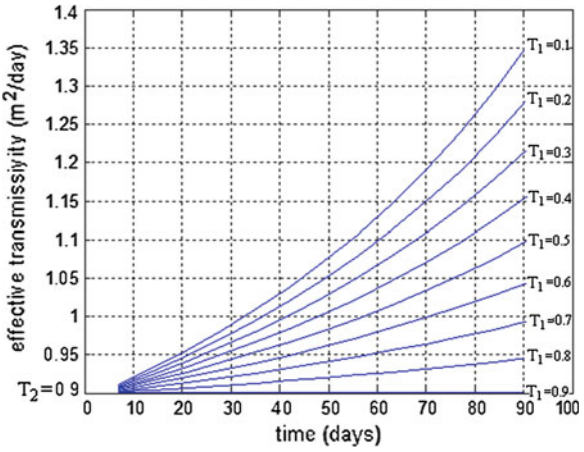

Fig. 9.6 Master *curves* for effective transmissivities for $T_2 > T_1$

days up to half of year had been a common practice in the Soviet Union. I had used those master curves always when it seemed to be appropriate. However I am not aware of somebody else who had been doing this.

Let us complicate the problem slightly. Namely, the hydrogeological process is the same as above with the same initial and boundary conditions but hydrogeological object comprises three geological bodies (Fig. 9.7). The "observations", that is, the results of solving the forward problem, are obtained at $x = 2L$. Interpretation model is homogeneous. The flow within each geological body is described by three equations

$$\frac{\partial h(x,t)}{\partial t} = A_j \frac{\partial^2 h(x,t)}{\partial x^2} \quad j = 1,\ 2,\ 3 \tag{9.43}$$

where x and t are the distance and time coordinates, $h(x,\ t)$ are the hydraulic head in intervals $[0,\ L]$ $(j = 1)$ and $[L,\ 3L]$ $(j = 2)$ and $[3L,\ 4L]$ $(j = 3)$ and $A_j = T_j/S$ is

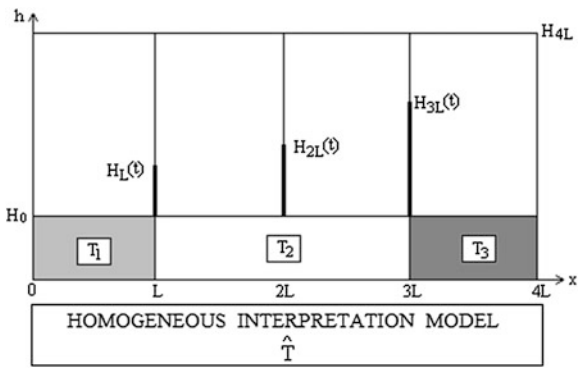

Fig. 9.7 Three-body confined aquifer and homogeneous interpretation model

the hydraulic diffusivity of body j, T_j is the hydraulic transmissivity of body j, and $S = 0.1$ is the storativity which is the same for all bodies. The initial and boundary conditions are the following:

$$h(x, 0) = 0, \quad 0 \le x \le 4L \tag{9.44}$$

$$h(0, t) = H_0 = 0 \quad \text{and} \quad h(4L, t) = H_{4L} = 1 \text{ m} \tag{9.45}$$

The inner boundary conditions on continuity of the hydraulic heads and the flux exist at $x = L$ and $x = 3L$:

$$\begin{aligned} &\lim_{x\to L}(h(x,t)) = \lim_{L\leftarrow x}(h(x,t)); \quad T_1 \lim_{x\to L}\frac{\partial h(x,t)}{\partial x} = T_2 \lim_{L\leftarrow x}\frac{(x,t)}{\partial x} \\ &\lim_{x\to L_3}(h(x,t)) = \lim_{L_3\leftarrow x}(h(x,t)); \quad T_2 \lim_{x\to 3L}\frac{\partial h(x,t)}{\partial x} = T_3 \lim_{3L\leftarrow x}\frac{\partial h(x,t)}{\partial x}. \end{aligned} \tag{9.46}$$

The explicit approximation of the hydraulic heads $h(2L,t_{i+1})$ can be presented as

$$\frac{h_{i+1} - h_i}{\Delta t} = \frac{T_2}{S}\frac{h_{3L,i} - 2h_i + h_{L,i}}{L^2}$$

where $h_i = h(2L,t_i)$, $h_{i+1} = h(2L,t_{i+1})$, $h_{L,i} = h(L\ t_i)$ and $h_{L,i} = h(3L,t_i)$, or

$$h_{i+1} \approx h_i + \frac{T_2 \Delta t}{SL^2}\left(h_{3L,i} - 2h_i + h_{L,i}\right). \tag{9.47}$$

It follows from the inner boundary conditions (Eq. 9.3.9 (9.46)) that

$$h_{L,i} = \frac{T_2}{T_1 + T_2}h_i, \quad h_{3L,i} = \frac{T_3 + T_2 h_i}{T_2 + T_3}. \tag{9.48}$$

Substituting the above results in Eq. 9.3.10 (9.47) yields the following procedure for making up the 'observations':

$$h_{i+1} \approx h_i + \frac{T_2 \Delta t}{SL^2}\left(\frac{T_3}{T_2 + T_3} + \left(\frac{T_2}{T_2 + T_3} + \frac{T_2}{T_1 + T_2} - 2\right)h_i\right). \tag{9.49}$$

The made-up 'observations' for one hundred days for the object with the hydraulic conductivities $T_1 = 0.1$, $T_2 = 0.2$ and $T_2 = 0.9$ m^2/day calculated by Eq. 9.49 are presented in Fig. 9.8.

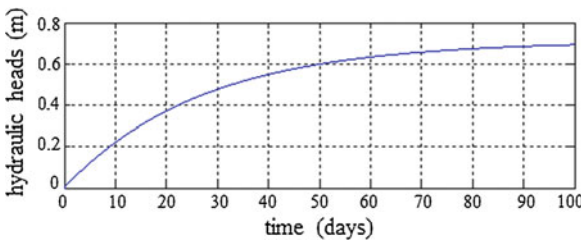

Fig. 9.8 Development of the hydraulic heads at $x = 2L$ during the first 100 days according to Eq. 9.49 ($T_1 = 0.1$, $T_2 = 0.2$ and $T_2 = 0.9$ m^2/day)

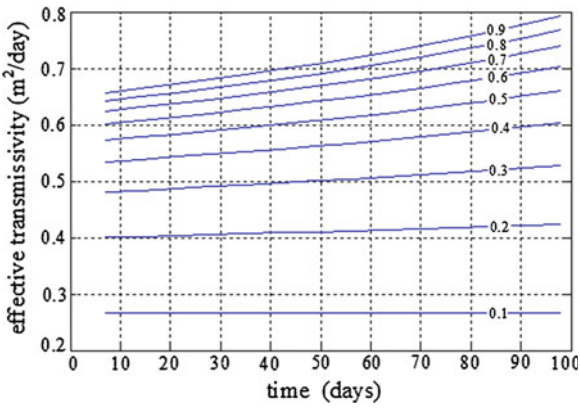

Fig. 9.9 Master *curves* obtained by the homogeneous interpretation model to the object presented in Fig. 9.8 with the hydraulic transmissivities $T_1 = 0.1$, $T_2 = 0.2$ m^2/day. Values of the transmissivities T_3 are shown on the pertinent plots

The effecting hydraulic transmissivity of the homogeneous model (Fig. 9.7) for the given structure of the geological object and the efficiency criterion ($\hat{h}_{i+1} = h_{i+1}$) can be calculated by equation applying implicit method this time:

$$\hat{T}_{i-1,i} = \frac{SL^2}{2(t_i - t_{i-1})} \ln \frac{1 - 2h_{i-1}}{1 - 2h_i}. \tag{9.50}$$

Masters curves in Fig. 9.9 are presented for the case when hydraulic conductivities $T_1 = 0.1$, $T_2 = 0.2$ m^2/day are fixed and hydraulic conductivity T_3 varies. The same curves can be made up for other combinations of $T_{1:3}$ and for objects with different numbers of geological bodies.

9.4 Conclusion

The transforming mechanisms can be applied to formulating and solving inverse problems related to underground flows. However they cannot eliminate the inherent incorrectness of those problems. When manifolds of the transforming mechanisms are created by the usage of different weightings, the incorrectness usually is caused by limited diversity of the weights assigned to the available observations. Whatever weights are applied, they are acting as if their values are interval [0, 1] or [−1, 1], if negative weights are applied. The failures can be caused also by unlucky choices of the models representing real geological object and monitoring networks providing not satisfactory amount or diverse data. Fortunately, the possibility of such failures can be found out before even starting the pertinent field investigations and taking in consideration in the stage of designing the pertinent projects. The projects can be corrected and optimized during their implementations based on incoming information. Thus the approach based on the transforming mechanisms permits obtaining the best results according to the

accepted definition of the 'best'. However, since our notions of geological objects are just models and, as such, false, the results of solving inverse problems are uncertain, meaning that their inaccuracy is impossible to evaluate in a provable way.

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Gorokhovski VM, Jazvin LS (1970) On evaluation of the hydraulic conductivity in multilayered aquifers (К вопросу определения коэффициентов фильтрации в многослойных водоносных горизонтах). In: Proceeding of VSGINGEO, vol 32. Moscow, pp 57–63 (in Russian)

Chapter 10
Advective Solute Transport Through Porous Media

As mentioned in Chap. 1, the mathematical models, recognized by professional community, yield usually satisfying approximations of reality. The model of convective-dispersive solute transport through porous media discussed in this chapter makes exclusion. This model is considered as classical or fundamental (Parker and van Genuchten 1984; Pasek et al. 2000; Delleur 2006). However, it often fails to reproduce long tails of breakthrough curves. The procedure suggested in this chapter provides more flexible and accurate reproducing those long tails and the breakthrough curves in general. It also permits more thorough interpretation of the observed data.

The chapter is written for the second edition of this book. To minimize changes in the text of the previous one, the whole discussion on solute transport through porous media is concentrated in this chapter which structure resembles in general the structure of the first edition. The chapter starts with analysis of the traditional approach to simulation solute transport in porous media based on convective-dispersive equation. The weak spot of this classical model, difficulty with reproduction of long tails of the observed breakthrough curves, can be overcome by exclusion from the classic model of the fictitious dispersion coefficient and the mean pore water velocity. Instead hydrodynamic dispersion should be included in simulation procedures directly. The transforming mechanisms are not forgotten, though they are not a main focus here.

10.1 On Classical Convective-Dispersive Model

10.1.1 First Versus Third Type of Boundary Condition at Inlet

At present the standard, classical or fundamental, approach to simulation of solute transport through porous media is based on convective-dispersive equation. In the case of one-dimensional transport, the equation takes form

V. Gorokhovski, *Effective Parameters of Hydrogeological Models*,
Springer Hydrogeology, DOI: 10.1007/978-3-319-03569-7_10,

$$\frac{\partial C(x,t)}{\partial t} = \frac{D}{R}\frac{\partial^2 C(x,t)}{\partial x^2} - \frac{U}{R}\frac{\partial C(x,t)}{\partial x} - \frac{\Lambda}{R}C(x,t) \tag{10.1}$$

where $C(x, t)$ is the solute concentration in pore water at location x and instant t; and the constants D, R, U and Λ represent the dispersion coefficient, the retardation factor, the mean pore water velocity and the degradation rate accounting for decay and linear interactions of the solute with the surroundings such, for example, as linear sorption and desorption. However, solutions to Eq. 10.1 are prone to yielding simulation breakthrough curves which do not represent well long tails of the observed curves. "Such discrepancy is often regarded as incongruous with the classical convective-dispersive equation, a view seemingly corroborated by the inability of certain solutions of this equation to fit observed breakthrough curves," write Parker and van Genuchten (1984). To mitigate the issue, they suggest assigning the third type, flux, boundary condition at the inlet ($x = 0$):

$$C_0|_{x=-0} = \begin{cases} C_0 \\ 0 \end{cases} = C(0_+) - \frac{D}{U}\frac{\partial C}{\partial x}\bigg|_{x=0_+}, \quad \begin{matrix} 0 < t \le T \\ t > T \end{matrix}, \tag{10.2}$$

instead of the first type boundary condition:

$$C_0|_{x=-0} = \begin{cases} C_0 \\ 0 \end{cases} = C(0_+), \quad \begin{matrix} 0 < t \le T \\ t > T \end{matrix}, \tag{10.3}$$

where $C_0|_{x=-0}$ is the solute concentration in the influent reservoir ($x \le 0$), usually constant, and $C(0_+)$ its concentration in pore water in the column at the boundary with the influent reservoir ($x \ge 0$), T is the duration of the pulse.

Equation 10.2 represents continuity of the flux concentration C_f at the inlet. C_f is defined as

$$C_f = C_r - \frac{D}{U}\frac{\partial C_r}{\partial x}, \tag{10.4}$$

where C_r is the resident concentration, the solute concentration in pore water, i.e., the concentration understood traditionally. For example, concentration C in Eq. 10.1 is the resident concentration. (Note, if solution in the influent reservoir is well mixed, $\partial C_0/\partial x = 0$ for $x \le 0$, then both concentrations represents the same entity). Parker and van Genuchten (1984) write: "Flux concentration may be interpreted physically as representing the mean of the microscopic fluid concentration weighted by their respective microscopic fluid velocities". Such interpretation seems confusing, at least for me, in particular since the flux concentration is not measurable (Kreft and Zuber 1978; Parker and van Genuchten 1984). In my opinion, Eq. 10.4 is rather a mathematical transformation. In the case discussed by Parker and van Genuchten (1984) this transformation permits converting equation written for the resident concentration

$$\frac{\partial C_r(x,t)}{\partial t} = D\frac{\partial^2 C_r(x,t)}{\partial x^2} - U\frac{\partial C_r(x,t)}{\partial x} \tag{10.5}$$

to an identical equation written in terms of the flux concentration, and the boundary condition of the third type (Eq. 10.2) expressing the flux concentration becomes the boundary condition of the first type for the equation in term of the flux concentration. However, such complete elimination of the resident concentration from equations is possible seldom. Solute transport through porous media is usually simulated in terms of the resident concentration. And since the flux concentration is not measurable, Parker and van Genuchten (1984) suggest its local calculating based on Eq. 10.4.

Batu (2006) writes that Brigham (1974), Kreft and Zuber (1978, 1979), Parker and van Genuchten (1984) emphasize that the distinction between these two forms of concentrations is of fundamental importance in order to stipulate boundary conditions appropriate for specific experimental solute detection modes. [According to Kreft and Zuber (1978) the existence of resident and flux concentrations makes up four specific experimental solute detection modes, meaning the type of input and output concentrations. If both input and output concentrations are resident than the mode is RR, if the input concentration is resident and the output one is flux, the mode is RF. Two other modes are FR and FF]. Parker and van Genuchten (1984) motivate the use of the flux boundary condition at inlets of experimental soil columns by the fact that the simulation breakthrough curves obtained under the first type boundary condition do not fit well the observed breakthrough curves. However, the issue is not resolved yet (Paseka et al. 2000; Delleur 2006; Dušek et al. 2007; Appuhamillage et al. 2010). This may mean that the flux boundary condition either does not work as they should according to Parker and van Genuchten (1984), or their suggestion is ignored or both. Nevertheless, Parker and van Genuchten continue holding that only the flux condition is correct at inlets (Batu et al. 2013). This makes it interesting to look more attentively at the mathematical and physical basis for their suggestion presented most completely, to my knowledge, by Parker and van Genuchten (1984).

Parker and van Genuchten (1984), demonstrate the properness of the third type boundary conditions at the inlet by integrating Eq. 10.5 in small intervals [0, $l/2$] within porous media ($x \geq 0$):

$$\int_{0_+}^{l/2} \frac{\partial C_r(x,t)}{\partial t} dx = \int_{0_+}^{l/2} \left(D \frac{\partial^2 C_r(x,t)}{\partial x^2} - U \frac{\partial C_r(x,t)}{\partial x} \right) dx$$
$$= D \left(\frac{\partial C_r(l/2,t)}{\partial x} - \frac{\partial C_r(0_+,t)}{\partial x} \right) - U(C_r(l/2,t) - C_r(0_+,t)) \tag{10.6}$$

Then they approach the upper limit of their integrals to zero: $0_+ \leftarrow l/2$. Since function $C_r(x, t)$ within the solution domain (the porous media), including its boundary at $x = 0_+$, must be continuous with respect to x and t, the result of the above integrating when l approaches zero ($0_+ \leftarrow l$) is trivial identity $0 \equiv 0$. Parker and van Genuchten (1984) recognize this for the most left integral equalizing it to

zero. Then they reorganize the remaining terms of Eq. 10.6 bringing the terms containing $l/2$ to the left part of the obtained equation:

$$U \lim_{0_+ \leftarrow l}(C_r(l/2,t)) - D \lim_{0_+ \leftarrow l}\left(\frac{\partial C_r(l/2,t)}{\partial x}\right) = UC_r(0_+,t) - D\frac{\partial C_r(0_+,t)}{\partial x} \tag{10.7a}$$

and now a peculiar manipulation follows. They change the direction from which l approaches zero from right, $0_+ \leftarrow l/2$, to left, $l/2 \rightarrow \_0$ and write

$$U \lim_{l \rightarrow 0_-}(C_r(l/2,t)) - D \lim_{l \rightarrow 0_-}\left(\frac{\partial C_r(l/2,t)}{\partial x}\right) = UC_r(0_+,t) - D\frac{\partial C_r(0_+,t)}{\partial x} \tag{10.7b}$$

Mathematically such change of direction is valid only, if limits exist, meaning that both limits, from right and left, are equal. Parker and van Genuchten (1984) do not discuss the existence of the limits in Eq. 10.7b. However, as follows from their text which I quote later, they understand that C_r experiences discontinuity at $x = 0$ and, therefore, the transition from Eq. 10.7a to b is mathematically incorrect. Note that physically both parts of Eq. 10.7a relate to the porous media. However, only the right part of Eq. 10.7b relates to the porous media, and its left part belongs to the influent reservoir. The solution in the reservoir ($x \leq 0$) is assumed well mixed, $(\partial C(l/2,t)/\partial x = 0)$ and $C_r(l/2,t) = C_f(l/2,t)$ for any l approaching zero from left, $l \rightarrow \_0$. So the result desired by Parker and van Genuchten (1984) is obtained. However, their way of treating mathematics deprives their conclusion of provability.

The physical explanation presented by Parker and van Genuchten (1984) misuses the notion of representative elementary volume REV, which they define as interval [0, $l/2$]. The property value characterizing a REV represents average properties of many heterogeneous elements within the REV. In this sense, REV has geological and mathematical (statistical) meaning and is used to represent, as if, a geological point, providing continuity of description of geological properties (Brown et al. 2000). However, when the volume of REV approaches zero, the REV loses its representativeness as the means of averaging. Besides some averaged geological characteristics, such as strength of soil (Bolotin 1969), hydraulic conductivity (Rats 1968; Gorokhovski 2012), and dispersion coefficient (Delleur 2006; Dispersion 2013) depend on volumes of the samples on which they are being evaluated.

Since the introduction of the flux boundary condition does not have a proper mathematical and physical basis, it is interesting to see practical results of application of the flux type boundary conditions. The example below has been presented by Batu (2010) promoting the use of the flux condition. He considers steady state solute transport described by equation

$$\frac{d^2C(x)}{dx^2} - \frac{U}{D}\frac{dC(x)}{dx} - \frac{R\Lambda}{D}C(x) = 0. \tag{10.8}$$

According to Batu (2010), Eq. 10.8 is identical for both resident, C_r, and flux, C_f, concentrations. The boundary condition at the inlet for the flux concentration is of the first type:

$$C_f(0_+) = C_0 = C_f(0_-), \tag{10.9a}$$

where C_0 is the solute concentration in the influent reservoir. The third type boundary condition at the inlet is assigned when Eq. 10.8 presented in terms of C_r:

$$C_r(0_+) - \frac{D}{U}\frac{dC_r(x)}{dx}\bigg|_{x=0_+} = C_0. \tag{10.9b}$$

The outlet is put at infinity where both, concentration or its first derivatives, are equal to zero.

The solutions to both problems according to Batu (2010) and Gorokhovski (2013) are

$$C_f(x) = C_0\, exp\left(\left(\frac{U}{2D} - \sqrt{\left(\frac{U}{2D}\right)^2 + \frac{R\Lambda}{D}}\right)x\right), \tag{10.10a}$$

$$C_r(x) = \frac{C_0}{\frac{1}{2} + \frac{D}{U}\sqrt{\left(\frac{U}{2D}\right)^2 + \frac{R\Lambda}{D}}}\, exp\left(\left(\frac{U}{2D} - \sqrt{\left(\frac{U}{2D}\right)^2 + \frac{R\Lambda}{D}}\right)x\right). \tag{10.10b}$$

Comparing them in a peculiar way, which I could not explain, Batu (2010) concludes that the solution obtained under the first type boundary condition "may significantly overestimate the degradation parameter value" (coefficient Λ). However, in reality the solutions presented by Eq. 10.10a and b are just scaled versions of each other:

$$C_f(x) = \left(\frac{1}{2} + \frac{D}{U}\sqrt{\left(\frac{U}{2D}\right)^2 + \frac{R\Lambda}{D}}\right)C_r(x) \tag{10.11}$$

If for evaluating Λ to use the ratios

$$ln\frac{C_f(x_j)}{C_f(x_i)} = ln\frac{C_r(x_j)}{C_r(x_i)} = (x_j - x_i)\left(\frac{U}{2D} - \sqrt{\left(\frac{U}{2D}\right)^2 + \frac{R\Lambda}{D}}\right), \tag{10.12}$$

the resulting value of Λ is the same for both types of the boundary conditions. Note also that plots of $(x, \ln(C_f(x)))$ and $(x, \ln(C_r(x)))$ are similar, just shifted with respect to each other, and have similar tails.

However, this is not all yet. The keynote of Batu (2010) is the mass balance at the inlet, as if, provided by the use of the third, flux, type boundary condition. This means that the entire mass of a solute enters the porous media in form of the flux

concentration. Then the resident concentration $C_r(0_+)$ must be equal to zero. According to Eqs. 10.10b and 10.11, this is not the case. Thus, the inlet boundary produces an additional mass of the solute somehow. It would be interesting to know from where the additional mass appears. Thus, Batu (2010) does not add anything in support of the use of the flux condition. Contrary, it rather puts doubts in its correctness and practical usefulness.

Parker and van Genuchten (1984) understood that their foundation for introduction of the flux boundary condition is lame. Indeed, solutions to equation of mathematical physics must be continuous at boundaries of the solution domain. However, in the case presented by Batu (2010) we have

$$\begin{aligned} & C_0 = C_f(\_0) \;=\; C_f(0_+) \;=\; C_r(\_0) \\ \text{and} \quad & C_0 = C_r(\_0) \;\neq\; C_f(0_+) + \frac{D}{U}\frac{\partial C_r}{\partial x}\bigg|_{x=0_+}, \end{aligned} \tag{10.13}$$

i.e., the resident concentration experiences discontinuity at the inlet if $\partial C_r/\partial x \neq 0$ at $x = 0_+$. Parker and van Genuchten (1984) write about the discontinuity appearing due to their introduction of the flux boundary condition: "The incongruity of a concentration discontinuity at the boundary….must be tempered by realization that calculated values have no physical relevance within $l/2$ of the boundary." They also cannot accept the assumption that $\partial C_r/\partial x = 0$ at $x = 0$ because its acceptance would mean "a loss of mass flux continuity." Parker and van Genuchten (1984) write: "Considering the indeterminant nature of the microscopic features of the boundary transition region, the least we can do is require that the basic condition of mass conservation be met by the boundary conditions." However, as demonstrated by Batu's (2010) example, the flux boundary condition at the inlet violates the law of mass conservation.

To conclude discussion on validity of the first or third type boundary conditions at the inlet, let us remember that all solute transport equations are equations of mass conservation which must hold at any point of the solutions domains. If the law of mass conservation is violated just at a point, the corresponding, as if, solution is not a solution. The solutions to solute transport equations must be continuous in space and time at all points of the solution domains. Consider the following imaginary experiment. Let the influent reservoir and the soil column be considered as a heterogeneous object. Then the inlet boundary between them becomes an inner boundary condition. At such boundary both, the solute concentration and the solute mass flux must be continuous. The necessity of sacrificing one of these continuities rests in the classical Eq. 10.1 itself which includes the fictitious dispersion coefficient, as if, compensating for hydraulic dispersion, the main factor responsible for creating long tails of the observed breakthrough curves, and the mean pore water velocity excluding hydraulic dispersion from the classical model.

10.1.2 On Dispersion Coefficient

Two parameters of Eq. 10.1 make it inadequate tool for simulating solute transport through porous media. The first is the mean pore velocity U. The second is the dispersion coefficient D. The use of the mean pore velocity excludes from simulation the real physical phenomenon called hydraulic dispersion. The phenomenon expresses itself in the fact that fluids have different velocities within porous media. The actual velocities depend not only on hydraulic gradients and permeability of the media but on sizes and shapes of the pores and fractures and locations of observation points respectively to their walls. The streamlines carrying solute with low actual water velocities are responsible for long tails of the observed breakthrough curves mainly.

The dispersion coefficient is defined as

$$D = D_M + \alpha_L U, \tag{10.14}$$

where D_M is the coefficient of molecular diffusion and α_L represents the longitude dispersivity. The dispersivity is an empiric parameter whose definition varies depending on the researchers. Delleur (2006) writes: "Dispersivity is a transport property that is relatively difficult to measure experimentally…. Values of the longitudinal dispersivity typically range from about 1 cm for packed laboratory columns, to about 5 or 10 cm for field soils." A few definitions of the dispersivity from Delleur (2006) are presented in Table 10.1 in which L is the reference distance, i.e., the distance form the inlet in one-dimensional case.

According to Parker and van Genuchten (1984) the dispersion coefficient defined by Eq. 10.14 is incorporated into Eq. 10.1 to represent "*the combined effect of diffusion and hydrodynamic dispersion* on transport." How the dispersion coefficient does this has been never explained, to my knowledge. "The combined effect" should be somehow related to the dispersivity α_L. One of the most recent and typical descriptions of the role which dispersivity, as a component of the dispersion coefficient, plays in the solute transport models can be found in Wikipedia (Dispersion 2013) where the unknown author writes: "Dispersivity is actually a factor which represents our *lack of information* about the system we are simulating. There are many small details about the aquifer which are being averaged when using a macroscopic approach (e.g., tiny beds of gravel and clay in sand aquifers), they manifest themselves as an *apparent* dispersivity. Because of this, α is often claimed to be dependent on the length scale of the problem—the dispersivity found for transport through 1 m^3 of aquifer is different than that for transport through 1 cm^3 of the same aquifer material."

Table 10.1 Few definitions of dispersivity according to Delleur (2006)

$\alpha_L = 0.0175L^{1.46}$	Neuman (1990)
$\alpha_L = 0.1L$	Gelhar et al. (1992)
$\alpha_L = 0.83(logL)^{2.414}$	Xu and Eckstein (1995)

The above quotation, as well all others explaining or introducing the dispersion coefficient and the dispersivity, elucidates nothing about why and how this fictitious property represents "our lack of information." And this is not surprising. If the dispersion coefficient would represent a real physical entity, all terms in its definition, Eq. 10.14, were of the same dimension. However, it follows from the definitions of the dispersivity in Table 10.1, that only one of them, given by Gelhar et al. (1992), is consistent with the theory of dimension (note that consistent does not mean true). Two others deprive Eq. 10.14 of any physical meaning. They are just ad hoc empiric parameters used to fit better the corresponding observations. The definition of Xu and Eckstein (1995) is most obvious in this respect: they use a dimension entity as an argument of logarithm.

The suggestion to exclude the dispersion coefficient from solute transport models is not anything new. U.S. EPA (1987) writes: "Generally, short-time tracer experiments in permeable material are affected almost exclusively by hydrodynamic dispersion. In contrast, the concentrations of natural tracers moving very slowly in highly heterogeneous materials are affected profoundly by molecular diffusion." "Short-time" in this sense is not only the tracer experiments but also most day-to-day practical problems.

By the way, Parker and van Genuchten (1984) write: "In general, the flux transformation of the convective-dispersive equation will be valid only for constant D." By its definitions, the fictitious coefficient D is not constant. This not only deprives any sense the discussion about the only correct type boundary conditions but put in doubt Eq. 10.1 itself.

10.2 Model of Advective Solute Transport Involving Hydrodynamic Dispersion

10.2.1 Introductory Examples

10.2.1.1 Piston Displacement

To feel better the role of hydrodynamic dispersion, let us start with the simplest model of the solute transport, the piston displacement, described by equation

$$\frac{\partial C_{U_i}(x,t)}{\partial t} = -U_i \frac{\partial C_{U_i}(x,t)}{\partial x} \tag{10.15}$$

where U_i is the constant actual pore water velocity along some set of streamlines and $C_{U_i}(x,t)$ the concentration of the solvent in the flow carried by the set. The initial condition for all sets is

$$C(x,0) = 0 \tag{10.16}$$

The boundary condition for all sets of streamlines is

$$C(0,t) = \begin{cases} C_0 & 0 < t \le T \\ 0 & t > T \end{cases} \tag{10.17}$$

where T is the duration of the pulse. The solution to the problem formulated by Eqs. 10.15–10.17 is being sought in domain $(0 < x < \infty) \times (0 < t < \infty)$ where $x = 0$ corresponds to the inlet boundary. The method of characteristics leads to the following solution:

$$C_{U_i}(x,t) = \begin{cases} 0, & t \le \frac{x}{U_i} \\ C_0, & \frac{x}{U_i} < t \le T + \frac{x}{U_i} \\ 0, & t > T + \frac{x}{U_i} \end{cases} \tag{10.18}$$

To obtain the breakthrough curve at some location x, we need to sum the results for all N sets of different velocities, taking into account the shares of the total flux carried by each of them

$$C(x,t) = \sum_{i=1}^{N} p_i C_{U_i}(x,t), \tag{10.19}$$

where p_i is the share, the weight, of the total flux carried by the set of streamlines having the actual pore water velocity U_i. The weights are not negative. When the shares of the flux carried with different actual pore water velocities do not experience superposition, as for example, in case of an instantaneous pulse, then the weights are summing to one. Then the weights provide equality:

$$\overline{U} = \sum_{i=1}^{N} p_i U_i \tag{10.20a}$$

where $\overline{U}$ is the mean pore water velocity. The above equality is actually the boundary condition of the first type for each set of streamlines carrying the flux with the actual pore water velocity U_i:

$$C_0 \overline{U} = C_0 \sum_{i=1}^{N} p_i U_i \tag{10.20b}$$

The condition provides continuity of the concentration and solute mass flux at the inlet. (In the case of continuous distributions of the actual pore water velocities, Eqs. 10.19 and 10.20a, b could be rewritten in the integral form). When pulse duration is finite, superposition of mass carried with different actual pore water velocities takes place. This case is discussed below in Sect. 10.2.2.

Figure 10.1 presents the results of simulation of the piston replacement of a tracer taking into account only the mean pore water velocity ($\overline{U} = 0.3367$ m/day) and calculated by Eqs. 10.18 and 10.19. The assigned distributions of the actual pore velocities and their weights are presented in Table 10.2. Duration of the pulse

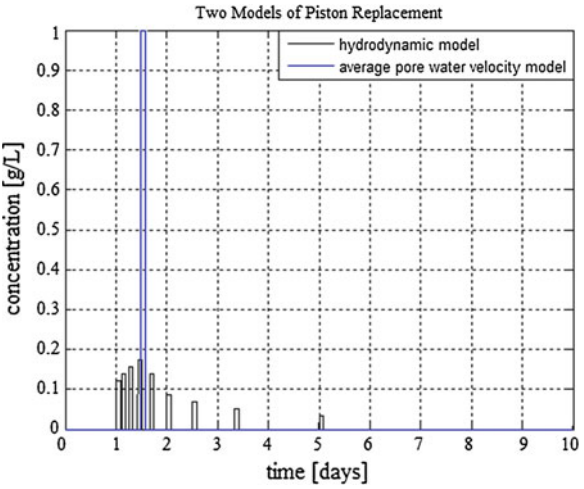

Fig. 10.1 Comparison of simulation breakthrough curves at the outlet ($x = L = 0.5$ m) for piston replacement with and without taking in consideration the hydrodynamic dispersion

is 2 h, its concentration, C_0, is 1 g/L, the length of the column, L, is 0.5 m. The velocity and the pulse duration are selected in a way to minimize superposition of the solute mass at the outlet. This permits equalizing the observed effluent concentrations to the weights and demonstrating that in the case of discrete distribution of pore water velocities, the periods may appear when the effluent concentrations of the tracer are equal to zero.

The envelope to the discrete concentrations in Fig. 10.1 could be interpreted as an approximation of the breakthrough curve caused by hydrodynamic dispersion. Its shape depends on distributions of the actual pore water velocities and shares of the total flux carrying by them. In the case of nonreactive tracers, only hydrodynamic dispersion stretches and makes breakthrough curves asymmetric. The stretching could be and usually is considerable. Thus, in the above example the pulse which duration is 2 h is passing the outlet boundary during 20 days and 2 h, i.e., 482 h. According to the standard piston model the solvent comes at the outlet at 1.4848 day and leaves the column at 1.5682 day. Only limitations on the duration of the experiments and the accuracy of concentration measurements do not permit observing actually very long tails of the breakthrough curve.

10.2.1.2 Transport of Solute Interacting with Surroundings Linearly

Let us add to Eq. 10.15 the term accounting for linear interaction between the solute and the surroundings:

$$\frac{\partial C_{U_i}(x,t)}{\partial t} = -\frac{U_i}{R}\frac{\partial C_{U_i}(x,t)}{\partial x} - \frac{\Lambda}{R}C_{U_i}(x,t). \tag{10.21}$$

Table 10.2 Pore water velocities U (m/day), arrival time L/U and leaving time $L/U + T$ (days), shares p of the total flux carried by corresponding U and effluent concentrations $C(L, t)$ (g/L)

U	0.5	0.45	0.4	0.35	0.3	0.25	0.2	0.15	0.1	0.05	0.025
L/U	1	1.1111	1.25	1.4286	1.6667	2	2.5	3.3333	5	10	20
$L/U + T$	1.0833	1.1944	0.1622	0.15119	1.75	2.0833	2.5833	3.4167	5.0833	10.083	20.083
p	0.1217	0.1391	0.1566	0.1739	0.1391	0.0870	0.0696	0.0522	0.0347	0.0174	0.0087
$C(L, t)$	0.1217	0.1391	0.1566	0.1739	0.1391	0.0870	0.0696	0.0522	0.0347	0.0174	0.0087

The initial and boundary conditions remain those presented by Eqs. 10.16 and 10.17. Then the solution to the problem formulated by Eqs. 10.21, 10.16 and 10.17 obtained by the method of characteristics is

$$C_{U_i}(x,t) = \begin{cases} 0, & t \le R\frac{x}{U_i} \\ C_0\, exp\left(-\Lambda\frac{x}{U_i}\right), & R\frac{x}{U_i} < t \le RT + R\frac{x}{U_i}. \\ 0, & t > RT + \frac{R}{U_i}x \end{cases} \tag{10.22}$$

The following data are assigned for the example below. The concentration of the pulse $C_0 = 1$ g/L; the pulse duration $T = 2$ h, the length of column $L = 0.5$ m and $\Lambda = 0.3$/day. The pore water velocities U_i are decreasing from 1 to 0.1 m/day with decrement -0.001 m/day. The lowest velocity is assigned equal 0.05 m/day. This choice of the pore water velocity is defined by the desire to make their distribution closer to continuous. The corresponding weights p_i are obtained as a series of the values from 10 to 0.99 decreasing with decrement -0.01 and then divided by their sum.

The results of solute transport simulation under the above conditions, the breakthrough curves at $x = 0.25$ m and at the outlet at $L = 0.5$ m, are presented in Fig. 10.2. The part of the breakthrough curve presented in Fig. 10.3 reveals also that the simulation pore water velocities are discrete. It is shown in Fig. 10.3 that there exist intervals in the breakthrough curves in which concentration of the solute is equal to zero. For example, the share of the solute carried with the velocity 0.1 m/day leaves the column at 7 h after beginning of the process, and the one carried with the velocity 0.05 m/day arrives at the outlet 3 h later. Thus, in interval [7, 10] h, the effluent has concentration equal to zero, but traces of the solute in the effluent could be found even after 10 h of the test.

The parts of the breakthrough curves at $x = 0.25$ and 0.50 m in time interval [0, 2] day are presented in Fig. 10.4. Both curves starts at the instant when the

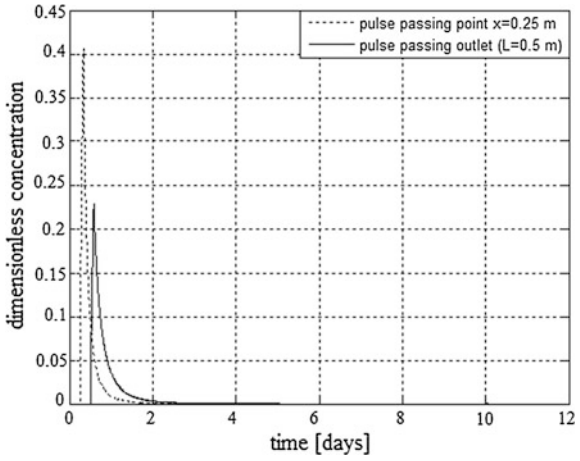

Fig. 10.2 Breakthrough curves at $x = 0.25$ and 0.5 m

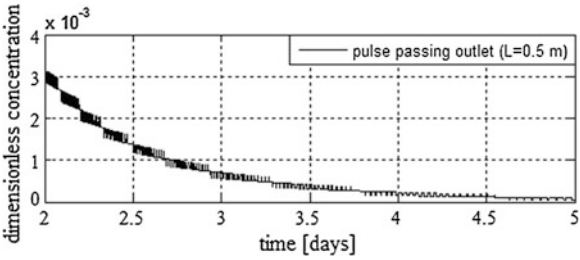

Fig. 10.3 Breakthrough curve at $x = 0.5$ m for time interval [2, 5] days

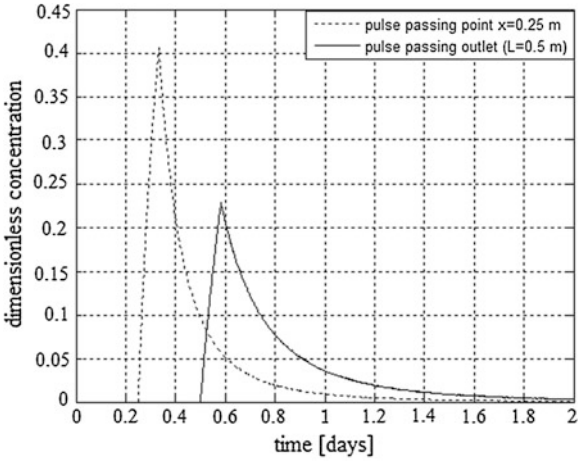

Fig. 10.4 Breakthrough curves at $x = 0.25$ and 0.5 m for time interval [0, 2] days

solute carried with the maximal velocity reaches the corresponding reference points ($t = 0.25$ and $t = 0.5$ day). At these moments concentration of the solute in the streamlines with the maximal actual pore water velocity is 0.9277 and 0.8607 g/L. All other streamlines do not bring the solute at the reference points yet. Thus, what has been brought is diluted by the total flux, multiplied by the corresponding weight, to the effluent concentrations 0.0019 and 0.0017 g/L.Then other streamlines started adding their shares of the solute and its concentration in the effluent grows, achieving at some instants its maximum, C (0.25, 0.333) = 0.4053 and C (0.5, 0.584) = 0.2281 g/L correspondingly. Then the concentration starts decreasing, since the streamlines with greater actual pore water velocity do not carry the solute.

10.2.2 Example of Simulation of Real Column Test

Practical application of the suggested advective solute transport simulation method involving directly hydraulic dispersion is demonstrated on the data published by Paseka et al. (2000). Their goal was testing the classical convective-dispersive

model in column tests with undisturbed and disturbed soils. They worked with three ionic tracers Cl^-, Br^- and K^+. The anions were considered to be nonreactive and traveling through the column without retardation, $R = 1$. Paseka et al. (2000) wrote that the K^+ ion was subjected to nonlinear adsorption and to cation exchange with Ca^{2+} and Mg^{2+}. However, they did not provide quantitative characteristics of the exchange. They applied only a pulse source to the column with undisturbed soil and pulse and continuous sources to the columns with disturbed soil. The breakthrough curves for the nonreactive tracers were in sufficient agreement with the simulation results only in the test with steady state solute transport in column of 3.5 cm length. Describing application of the pulse source which lasted 2.39 min to the column of 36 cm length with undisturbed soil, Paseka et al. (2000) wrote: "Comparison of experimental breakthrough curves of all tracers with numerical solution indicates that it could not adequately describe the transport of ions. Both Cl^- and Br^- were expected to first reach their initial concentrations and then drop sharply…. Instead, their concentrations reached only about 70 % of the originally introduced concentrations. In addition, the K^+ peak was approximately four times lower than the given by numerical solution" (see Fig. 10.5). In the experiments with durations of pulses 78.7 and 74.7 h with disturbed soils in columns of 15 cm length, they obtained good agreements of the observed and simulation breakthrough curves for their ascending parts for both Cl^- and Br^-. However, the descending parts of the simulation breakthrough curves are inadequate to the observed ones. Paseka et al. (2000) state that their K^+ transport simulation was a complete failure in all their column experiments. (For unexplained reasons, they, likely, used the piston replacement model, simulating the K^+ transport through the undisturbed soil).

The data on the column test conducted by Paseka et al. (2000) with the undisturbed soil and on simulation of the K^+ transport with the direct use of hydrodynamic dispersion are presented in Table 10.3. Their data do not suit requirements of the suggested method in full. Thus, the first measurement of the solute concentrations was made at 1 min from the beginning of the experiment. The measured concentrations of the nonreactive tracers in the effluent at that instant were high enough, meaning that maximal pore water velocity remained unknown and is, likely, considerably higher than its mean value. The pulse duration 2.39 min for the mean pore water velocity 36 cm/min in the column of 36 cm length was relatively long and led to superposition at the outlet of the

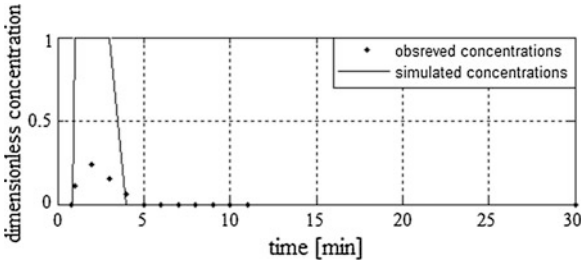

Fig. 10.5 Simulation and observed breakthrough curves of K^+ in the experiment with undisturbed soil according to Paseka et al. (2000, Fig. 4)

Table 10.3 Comparison of concentrations of K^+ ion observed by Paseka et al. (2000) in test with the undisturbed column 1 and simulated by Eq. 10.24

Time (min)	Paseka et al. (2000)						Eq. 10.23	
	Cl^-		Br^-		K^+		U	K^+
	(mg/L)	C/C_0	(mg/L)	C/C_0	(mg/L)	C/C_0	(cm/min)	C/C_0
1	111.79	0.47	186.11	0.48	53.37	0.11	36	0.2377
2	191.87	0.71	241.82	0.63	114.79	0.24	18	0.2387
3	166.33	0.62	257.85	0.67	72.99	0.15	12	0.1209
4	73.85	0.27	152.59	0.4	29.34	0.06	9	0.0305
5	25.52	0.09	56.85	0.15	nd	0	7.2	0.0059
6	18.63	0.07	42.72	0.11	nd	0	6	0.0027
7	12.12	0.04	29.48	0.08	nd	0	5.1429	0.0009
8	8.19	0.03	21.73	0.06	nd	0	4.5	0.0004
9	6.14	0.02	17.73	0.05	nd	0	4	0.0002
10	4.71	0.02	14.88	0.04	nd	0	3.6	0.0001
11	4.97	0.02	12.85	0.03	nd	0	3.2727	0.0000
30	0.11	0	5.32	0.01	nd	0	1.2	0.0000

[Initial concentrations C_0: 270.37 (Cl^-), 384.17 (Br^-), 486.15 (K^+); mg/L]

tracers' masses carried with different pore water velocities, making it difficult to find the weights corresponding to the particular velocities. (Some suggestions on better column test methodology for the approach being discussed are mentioned in Sect. 10.4). However, the conditions close to ideal are rare, if ever, met in practical applications. The discussed example permits demonstrating the way around which, probably, can work in many, if not all, circumstances.

Let us calculate the concentration which is not equal to zero based on Eq. 10.22 which for $x = L$ take form

$$C_{U_i}(L,t) = C_0 exp\left(-\Lambda \frac{L}{U_i}\right) = C_0 exp(-\Lambda t_i), \quad \frac{R}{U_i}x < t \le RT + \frac{R}{U_i}x \tag{10.23}$$

where t_i is the observed arrival time at the outlet at $x = L$. Since the pulse has a finite duration, the concentration observed at this instant is superposition of the solute concentration carried by the streamlines which actual pore water velocities make up some interval including U_i. The corresponding dimensionless concentrations of nonreactive tracers Cl^- and Br^- can be interpreted as apparent weights $p_i^{(a)}$, corresponding to velocity U_i. Since different streamlines with different velocities arrive simultaneously at the outlet, their sum naturally exceeds one and for this reason I call these weights apparent. Then Eq. 10.19 can be rewritten as

$$C(L,t_i) = p_i^{(a)} C_{U_i}(L,t_i), \tag{10.24}$$

In this example the apparent weights correspond to the dimensional concentrations of Cl^-, though concentrations of Br^- or some their combination could be

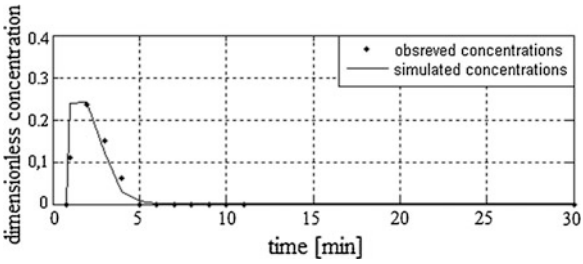

Fig. 10.6 K^+ ion transport through undisturbed soil column. Results presented by Paseka et al. (2000) and simulated by Eqs. 10.23 and 10.24 with degradation rate $\Lambda = 0.546$/min

applied as well. The values of the simulation concentration of the K^+ ion are presented in the last column of Table 10.3. The arrival time of the K^+ ion carried with the fastest pore water velocity is assigned arbitrary as 0.8 min. This corresponds to the pore water velocity 45 cm/min.

The concentrations observed by Paseka et al. (2000) and calculated by Eq. 10.24 with direct involvement of hydrodynamic dispersion are presented in Fig. 10.6. The later are obtained with coefficient $\Lambda = 0.546$/min which is found by the trial and error method. Comparison of the results presented in Figs. 10.5 and 10.6 demonstrates clearly the advantage of the suggested approach.

10.3 Transforming Mechanisms for Degradation Rate

10.3.1 Estimating Hydraulic Dispersion

The explicit incorporation of the hydrodynamic dispersion in formulation of solute transport simulation requires preliminary resolving of two issues. First is estimation of the actual pore water velocities. The second is estimation of the weights, the shares of the total flux carried by different actual water pore velocities. Both properties can be evaluated by direct observations on breakthrough curves in the experiments with nonreactive tracers.

Conceptually, the most obvious and theoretically pure way of evaluation of the actual pore water velocities and the corresponding weights is conducting experiments with nonreactive tracer steady state transport. An example of a possible breakthrough curve in this case is presented in Fig. 10.7: the tracer is carried with each velocity all the time and the breakthrough curve becomes an analog of a cumulative distribution function from the theory of probability. Based on this curve, a function of the density actual pore water velocity, analog of the probability density function (pdf), can be obtained. Concentrations of the tracer corresponding to different velocities are the shares of the flux carried with corresponding velocities.

Another way of finding distribution of the pore water velocities and the pertinent weights is the use of instant pulses of tracers. In this case the pulse passes the

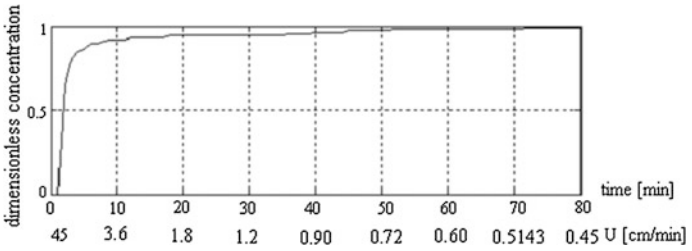

Fig. 10.7 Possible steady state breakthrough curve for nonreactive tracer in Paseka et al. (2000) experiment with undisturbed soil

outlet instantly which exclude superposition of the tracer's mass. If it had been possible to make the pulse duration as well as sampling of effluent concentrations instantaneous, it would be possible to find all the actual pore water velocities and their weights even for the actual pore water velocity changing continuously. The results shown in Fig. 10.8 are obtained by simulation of a tracer injected by the pulse whose duration is 0.001 min. The actual pore water velocities in this case are selected in the way excluding superposition of the tracer masses which is not difficult considering that duration of the pulse. Figure 10.8 represents factually a specter of the concentrations corresponding to the simulated pore water velocities from which those velocities could be evaluated. (Reactive tracers can be used also for evaluation of the actual water pore velocities and their weights. However, their use makes more complicated interpretation of the observations, since the interpretation requires knowledge of the parameters and mechanisms of interaction of the tracers with surrounding).

Thus, the experiments with transport of nonreactive tracer could be considered as the method of evaluation of hydrodynamic dispersion. However, both steady state regime and instant pulse of the tracer could be not acceptable practically. Then the use of the apparent weights, described in Sect. 10.2.2 is, likely, the best practical way to deal with hydrodynamic dispersion. It is also important to fix the first appearance of tracers in the effluent for evaluating the maximal pore water velocity.

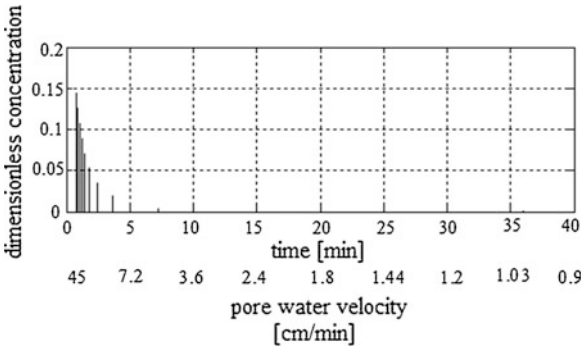

Fig. 10.8 Simulated specter of the concentrations, weights, carried by different pore water velocities when duration of pulse of nonreactive tracer is 0.001 min

10.3.2 Estimating Effective Value for Degradation Rate for Homogeneous Model

Let as assume that the superposition of the solute mass carried by the sets of streamlines with different actual pore water velocities is absent. Then the effective concentrations different from zero at the instant $t_i = L/U_i$ can be presented based on Eqs. 10.23 and 10.24 as

$$\widehat{C}_{U_i}(L,t_i) = p_i C_0 exp\left(-\widehat{\Lambda}\frac{L}{U_i}\right) = p_i C_0 exp\left(-\widehat{\Lambda}t_i\right) \tag{10.25}$$

where $\widehat{\Lambda}$ is the unknown rate of degradation and t_i is the time when the solute carried with the actual pore velocity water U_i reaches $x = L$. Taking the natural logarithms of Eq. 10.25 we obtain:

$$ln\frac{\widehat{C}_{U_i}(L,t_i)}{p_i C_0} = -\widehat{\Lambda}t_i \tag{10.26}$$

If we have N observations on $C_i(L, t_i)$, the effective value of $\widehat{\Lambda}$, can be obtained by the least square method by minimization of the sum

$$s = \sum_{i=1}^{N}\left(\widehat{\Lambda}t_i - ln\frac{C_{U_i}(L,t_i)}{p_i C_0}\right)^2 \tag{10.27}$$

The standard technique of the least square method yields

$$\sum_{i=1}^{n}\left(t_i ln\frac{C_{U_i}(L,t_i)}{p_i C_0}\right) = -\widehat{\Lambda}\sum_{i=1}^{N}t_i^2 \tag{10.28}$$

and finally

$$\widehat{\Lambda} = -\frac{\sum_{i=1}^{N}\left(t_i ln\frac{C_{U_i}(L,t_i)}{p_i C_0}\right)}{\sum_{i=1}^{N}t_i^2} \tag{10.29}$$

It is easy to check that if the homogeneous model represents the object which is really homogeneous and the observations and calculations are executed without errors, then $\widehat{\Lambda} = \Lambda$. Indeed substituting in Eq. 10.26 $C_i(L, t_i)$ instead of $\widehat{C}_{U_i}(L,t_i)$, we obtain

$$\widehat{\Lambda} = -\frac{\sum_{i=1}^{N}\left(t_i ln\frac{C_{U_i}(L,t_i)}{p_i C_0}\right)}{\sum_{i=1}^{N}t_i^2} = \Lambda\frac{\sum_{i=1}^{N}t_i^2}{\sum_{i=1}^{N}t_i^2} = \Lambda \tag{10.30}$$

In the case of data carrying errors the effective parameter can differ from the actual one. Besides to make the problem easier, Eq. 10.25 is linearized by taking logarithms. Consequently the effective degradation optimizes logarithms of the

concentrations, not the concentrations themselves. As Eq. 10.30 shows, this does not matter, if our model represents the object exactly and calculations are accurate. However, if the model is not true, such linearization yields worse results than the results of the trial and error method, and the simulated breakthrough curves based on them could be biased more or less, i.e., shifted with respect to observations. It should be noted also that the logarithm of zero does not exists and Eq. 10.27 cannot include zero concentrations.

Though the difference between the results obtained by Eq. 10.29 ($\Lambda = 0.463$/min) and by the trial and errors method ($\Lambda = 0.546\ \text{min}^{-1}$) can be considered as acceptable practically, the use in simulation of $\Lambda = 0.463$/min leads to some shift of the simulation results (Fig. 10.9). The results are obtained on the data presented by Paseka et al. (2000) on the observation on the ion K^+ transport in their experiment with the column of undisturbed soil (Table 10.3). Nevertheless, the reproduction of the breakthrough curve with degradation rate obtained by Eq. 10.29 is much better than that obtained by Paseka et al. (2000).

10.3.3 Solute Transport Through Piecewise Heterogeneous Porous Media

Let us consider one-dimensional solute transport through porous media in which at location x_1 coefficient Λ experiences discontinuity changing from Λ_1 to Λ_2. The actual water pore velocities $U_{1:N}$ and their weights $p_{1:N}$ are known. The goal is simulation of the breakthrough curve at $x = L(L > x_1)$.

The breakthrough curve at x_1 makes up the boundary condition for interval $(x_1, L]$. The solute concentrations brought at x_1 by the ith set of streamlines are described by Eq. 10.24 where x_1 substitutes for L and Λ_1 for Λ. Then the breakthrough curve at x_1 can be obtained as

$$C(x_1, t) = \sum_{i=1}^{N} p_i C_{U_i}(x_1, t) \tag{10.31}$$

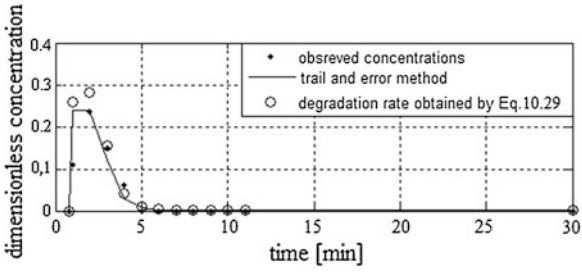

Fig. 10.9 K^+ ion transport: results presented by Paseka et al. (2000) and simulated by Eqs. 10.23 and 10.24 with degradation rate $\Lambda = 0.546$/min and obtained by least square method ($\Lambda = 0.463$/min, Eq. 10.29)

The solution for the concentrations carried by the ith and not equal to zero within interval $(x_1, L]$ is

$$C_{U_i}(L,t) = C\left(x_1, t - R\frac{x_1}{U_i}\right) exp\left(-\Lambda_2 \frac{L - x_1}{U_i}\right) \tag{10.32}$$

Since the first right hand multiplier in Eq. 10.32 represents the concentration at x_1 for interval $(0, x_1)$, Eq. 10.32, we can write

$$C_{U_i}(L,t_i) = p_i C_0 exp\left(-\Lambda_1 \frac{x_1}{U_i}\right) exp\left(-\Lambda_2 \frac{L - x_1}{U_i}\right) \tag{10.33a}$$

or

$$C_{U_i}(L,t_i) = p_i C_0 exp\left(-\Lambda_1 t_i^1\right) exp\left(-\Lambda_2 \left(t_i - t_i^1\right)\right) \tag{10.33b}$$

where t_i^1 is the travel time of the solute from the inlet to the boundary at $x = x_1$ and t_i is its traveling time to the outlet at $x = L$. Summing the above solutions for each set for streamlines, we finally obtain

$$C_{U_i}(L,t_i) = \sum_{i=1}^{N} p_i C_0 exp\left(-\left(\Lambda_1 \frac{x_1}{U_i} + \Lambda_2 \frac{L - x_1}{U_i}\right)\right) \tag{10.34a}$$

or

$$C(L,t_i) = \sum_{i=1}^{N} p_i C_0 exp\left(-\left(\Lambda_1 t_i^1 + \Lambda_2 \left(t_i - t_i^1\right)\right)\right) \tag{10.34b}$$

where N is the number of different actual pore water velocities. Solutions for greater number of piecewise interval can be obtained in the same way.

10.3.4 Transforming Mechanisms for Degradation Rate and Inverse Problem Solving

Let a porous media be piecewise homogeneous in sense of the degradation rate, i.e., it consists of two homogeneous bodies with boundary between them at $x = x_1$. The degradation rates of the bodies are Λ_1 and Λ_2 correspondingly. However, their values are not known and the goal is to evaluate them using observations on the breakthrough curve at $x = L$.

Let us start with linearization of the solution presented by Eq. 10.33b by taking the natural logarithm of its both terms

$$ln(C_{U_i}(L,t_i)) = ln(p_i C_0) - \left(\Lambda_1 t_i^1 + \Lambda_2 \left(t_i - t_i^1\right)\right) \tag{10.35}$$

For the homogeneous model the same procedure leads to equation

$$ln\left(\widehat{C}_{U_i}(L,t_i)\right) = ln(p_i C_0) - \widehat{\Lambda}_{1:N} t_i \tag{10.36}$$

where N is the number of observations on the breakthrough curve at $x = L$ taken in account for evaluation of the effective degradation rate $\widehat{\Lambda}_{1:N}$. To find it, we need to minimize the sum

$$s = \sum_{i=1}^{N} \left(ln\left(\widehat{C}_{U_i}(L,t_i)\right) - ln(C_{U_i}(L,t_i))\right)^2. \tag{10.37}$$

Substituting in Eq. 10.37 the corresponding Eqs. 10.36 and 10.35 and applying the list square method, we obtain the transforming mechanism

$$\widehat{\Lambda}_{1:N} = w_{1,1:N}\Lambda_1 + w_{2,1:N}\Lambda_2 \tag{10.38a}$$

with the affecting factors

$$w_{1,1:N} = \frac{\sum_{i=1}^{N} t_i t_i^1}{\sum_{i=1}^{N} t_i^2} \quad \text{and} \quad w_{2,1:N} = \frac{\sum_{i=1}^{N} \left(t_i - t_i^1\right) t_i}{\sum_{i=1}^{N} t_i^2} \tag{10.38b}$$

which sum, as expected, is equal to one to one.

As discussed in the previous chapter, there are different ways of formulating and solving the inverse problem, i.e., evaluating values of the governing parameters of models based on available data. The simplest way to find the degradation rates Λ_1 to Λ_2 seems to be calculating the transforming mechanisms for two distinguished sets of observations on the breakthrough curve. The second sent obtained by the use of K observations yields the second transforming mechanism:

$$\widehat{\Lambda}_{1:K} = w_{1,1:K}\Lambda_1 + w_{2,1:K}\Lambda_2 \tag{10.39}$$

which with the mechanism presented by Eq. 10.38a make up system comprising two equations for two unknowns. The corresponding effective degradation rates can be evaluated by the trial and error method or by Eq. 10.30.

Note, that the weights $p_{1:N}$ and $p_{1:K}$ are assumed to be apparent like those used in the example of Sect. 10.2.2.

10.4 Conclusions

Inability of the solutions to the classical convective-dispersive equation, Eq. 10.1, to fit long tails of the observed breakthrough curves is the evidence of its incongruousness indeed. Asymmetry of the curves is caused mainly by the hydrodynamic dispersion. The constant mean pore velocity eliminates it from the model, and the fictitious dispersion coefficient introduced into Eq. 10.1, as well as in the

definition of the flux concentration, does not create any mechanisms compensating for hydrodynamic dispersion. Only for very low pore water velocities, diffusion starts playing role which could be comparable with advective solute transport. In such cases, diffusion should be presented in Eq. 10.1 as coefficient of molecular diffusion (U.S. EPA 1987).

The use of Eq. 10.21 applied to different actual pore water velocities, seems sounder and better physically grounded than the use of the classical convective-dispersive Eq. 10.1. The flexibility and the ability of the solution to Eq. 10.21 to fit the asymmetric breakthrough curves is the obvious evidence of its advantage over Eq. 10.1. Solving Eq. 10.1 in column tests requires knowledge conditions at both, inlet and outlet. Although the observed breakthrough curves present boundary conditions at the outlets, analytical solutions to Eq. 10.1 for column of finite length are expressed by infinite series. They are inconvenient and difficult for interpretation of the observed breakthrough curves. For this reason, solving Eq. 10.1, the second boundary condition is put in infinity which causes errors. Contrary, Eq. 10.21, to be solved, requires only one boundary condition. The controlled boundary condition at the inlet is sufficient. Equation 10.21 is the partial differential equation of the first order. This simplifies the solving solute transport problems and permits obtaining analytical solutions in many cases when its coefficients R, U and Λ are functions of time and/or distance. For example, if the actual pore velocity varies, $U_i = U_i(x)$, where x is the distance along a streamline, the solute transport is described by equation

$$R\frac{\partial C_{U_i}(x,t)}{\partial t} = -\frac{\partial (U_i(x)C_{U_i}(x,t))}{\partial x} - \Lambda C_{U_i}(x,t), \tag{10.40}$$

The solution to it under the initial and boundary conditions presented by Eqs. 10.16 and 10.17 is

$$C_{U_i}(x,t) = \begin{cases} 0, & t \le R\int\limits_0^x \frac{dx}{U_i} \\ C_0 exp\left(-(\Lambda + dU_i/dx)\int\limits_0^x \frac{dx}{U_i}\right), & t - R\int\limits_0^x \frac{dx}{U_i} \le T \\ 0, & t - R\int\limits_0^x \frac{dx}{U_i} > T \end{cases} \tag{10.41}$$

Another example: Paseka et al. (2000) mention that the K^+ ion was subjected to nonlinear adsorption and to cation exchange with Ca^{2+} and Mg^{2+}. Let us assume that one of these processes is linear and the other is nonlinear, and that nonlinear is proportional to concentration in some power α. Then the solute transport can be described by equation, presenting a mixed model:

$$R\frac{\partial C_{U_i}}{\partial t} = -U_i\frac{\partial C_{U_i}}{\partial x} - \Lambda C_{U_i} - \Lambda_\alpha C_{U_i}^\alpha, \tag{10.42}$$

where U_i is constant as well as parameters α and Λ_α governing by nonlinear interaction with the surroundings. Parameter α describes order of the nonlinear interaction. The dimension and physical meaning of Λ_α depend on parameter α. Parameter α is dimensionless, $[\alpha] = 1$. Since dimensions of all terms comprising Eq. 10.42 must be the same, then

$$[\Lambda_\alpha] = \left[R\frac{\partial C_{U_i}}{\partial t}\right] = \frac{\mathrm{ML}^{-3}\mathrm{T}^{-1}}{\mathrm{M}^{\alpha}\mathrm{L}^{-3\alpha}} = \mathrm{M}^{1-\alpha}\mathrm{L}^{-3(1-\alpha)}\mathrm{T}^{-1} = \left[\mathrm{C}^{1-\alpha}\right]\mathrm{T}^{-1}, \quad (10.43)$$

where M, L and T are the dimensions of mass, length and time respectively. The retardation factor R is dimensionless, $[R] = 1$. Thus, Λ_α define the rate of changing of values C^{1-a}.

Equation 10.42 is integrated in domain $(0 < x < \infty) \times (0 < t < \infty)$, where $x = 0$ corresponds to the inlet boundary, under the initial and boundary conditions given by Eqs. 10.16 and 10.17. The yielded nonzero solute concentrations carried by the streamlines whose actual flow velocity is U_i with flow are described by equation

$$C_{U_i} = C_0 e^{-\Lambda\frac{x}{U_i}}\left(1 + \frac{\Lambda_\alpha}{\Lambda}\left(1 - e^{-(\alpha-1)\Lambda\frac{x}{U_i}}\right)C_0^{\alpha-1}\right)^{-\frac{1}{\alpha-1}}, \quad R\frac{x}{U_i} < t \le RT + R\frac{x}{U_i} \quad (10.44)$$

The breakthrough curve obtained by application of Eq. 10.44, with summation prescribed by Eq. 10.24, to the data of Paseka et al. (2000) on the test with the undisturbed soil column is presented in Fig. 10.10. The figure shows that the mixed linear-nonlinear model with parameters $\alpha = 1.1$, $\Lambda = 0.546/\mathrm{min}$, $\Lambda_\alpha = 0.1\ \mathrm{mg}^{-0.1}\ \mathrm{cm}^{0.3}\ \mathrm{min}^{-1}$ reproduces the observed actual concentrations satisfactory. However, it may happen that a different set of the parameters or another kind of interaction between the solute and surroundings could do the same or even better job. The simulation results obtained by the linear and mixed model based on the data of Paseka et al. (2000) are presented in Fig. 10.11. They are undistinguishable practically. This means that speculations on which, if any, of the well working sets of the parameters is true are fruitless without understanding of the mechanisms of competing kinds of the interactions.

To distinguish between linear and nonlinear interactions of solute with surroundings, the experiments must be conducted with different boundary concentrations C_0. This does not change the dimensionless concentration in the case of the linear interaction. If the interaction is nonlinear, the difference between the dimensionless concentrations obtained for different C_0, depends on the governing parameters of the interaction. If this difference is not considerable, as in the case presented in Fig. 10.11, it is naturally to assume that the nonlinearity, if exists, is not essential. In the case of nonlinear interactions the changing may be considerable (see Fig. 10.12). The main factor of such changes is the order of interaction α, though the other governing parameters affect them also.

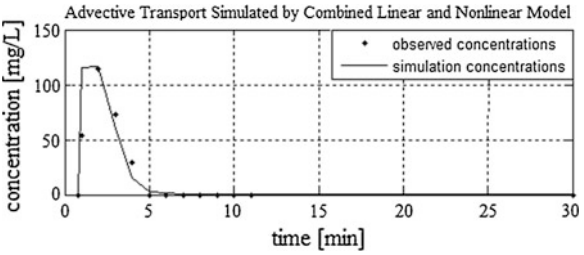

Fig. 10.10 K^+ ion transport: results presented by Paseka et al. (2000) and simulated by Eqs. 10.44 and 10.24 with parameter values $\alpha = 1.1$; $\Lambda = 0.546/\text{min}$; $\Lambda_\alpha = 0.1\ \text{mg}^{-0.1}\ \text{cm}^{0.3}\ \text{min}^{-1}$

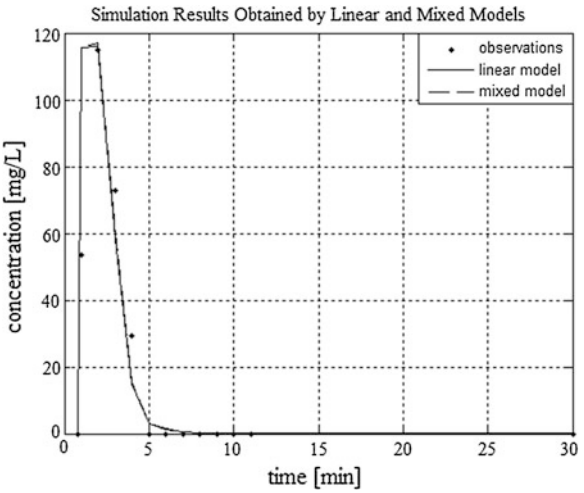

Fig. 10.11 Comparison based on the data of Paseka et al. (2000) the simulation results obtained by linear model, Eqs. 10.23 and 10.24, and mixed one, Eqs. 10.44 and 10.24

It follows from the ratio

$$\frac{C_{01U_i}}{C_{02U_i}} = \left(\frac{1 + \frac{\Lambda_\alpha}{\Lambda}\left(1 - e^{-(\alpha-1)\Lambda\frac{x}{U_i}}\right) C_{01}^{\alpha-1}}{1 + \frac{\Lambda_\alpha}{\Lambda}\left(1 - e^{-(\alpha-1)\Lambda\frac{x}{U_i}}\right) C_{02}^{\alpha-1}} \right)^{-\frac{1}{\alpha-1}} \tag{10.45}$$

where C_{01} and C_{02} are the boundary condition concentrations, and C_{01U_i} and C_{02U_i} are the corresponding dimensionless concentrations delivered at (x, t) by the streamlines carrying the solvent with the actual pore water velocity U_i. Then the equation follows

$$\left(\frac{C_{1U_i}(x,t)}{C_{2U_i}(x,t)}\right)^{(\alpha-1)} - \frac{1 + \frac{\Lambda_\alpha}{\Lambda}\left(1 - e^{-(\alpha-1)\Lambda\frac{x}{U_i}}\right)}{1 + \frac{\Lambda_\alpha}{\Lambda}\left(1 - e^{-(\alpha-1)\Lambda\frac{x}{U_i}}\right)} = 0 \tag{10.46}$$

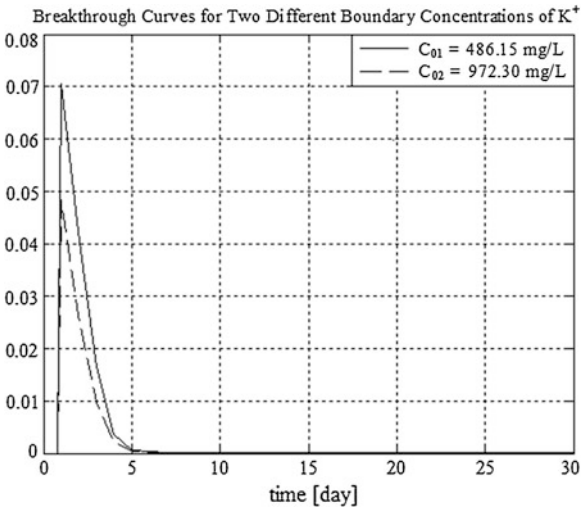

Fig. 10.12 Breakthrough curves simulated by mixed, Eqs. 10.44 and 10.24, for two different boundary condition C_{01} and C_{02} and $\alpha = 1.5$; $\Lambda = 0.546/\text{min}$; $\Lambda_\alpha = 0.1\ \text{mg}^{-0.5}\ \text{cm}^{1.5}\ \text{min}^{-1}$

where $C_{1U_i}(x,t)$ and $C_{2U_i}(x,t)$ are the actual concentration corresponding to the velocity U_i. Using different arrival times (x/U_i) we obtain the system of equations to find three unknown (α, Λ, Λ_α). To solve it is not an easy task but is possible still. The knowledge of one or two unknowns could be very helpful.

However, working with nonlinear or mixed models, one must be careful. Thus, when $\alpha = 1$, Eq. 10.44 experiences discontinuity, though it seems to be removable. For $\alpha < 1$, physically incorrect (growing with the time passing, negative and imaginary) concentrations can and will appear. I am not competent to explain in physical and chemical terms whether such values of α are realistic. If they are, then different models are needed to be worked out with this sort of solute transport problems.

The last example which I wish to present returns us to the linear advective solute transport model with the constant governing parameters, Eq. 10.21. However, at this time the initial condition is nonzero, and the boundary condition is zero:

$$C(x,0) = f(x) \tag{10.47}$$

$$C(0,t) = 0 \tag{10.48}$$

The solution to this problem for the solute carried by the streamlines with the actual pore velocity U_i is

$$C_{U_i}(x,t) = f\left(x - \frac{U_i t}{R}\right) exp\left(-\frac{\Lambda}{R}t\right) \tag{10.49}$$

The total solute concentration $C(x, t)$ can be obtained by summing with pertinent weights the concentrations provided by streamlines with different actual pore water velocities, Eq. 10.19. This last example shows that advective solute transport models with nonzero initial conditions, like this one, can be simple and flexible instrument in planning groundwater restoration and protection programs.

All problems in this chapter are one-dimensional. This is done in part to make presentation of the suggested approach simple and transparent. Nevertheless, the advective transport along streamlines is one-dimensional. To obtain two- and three-dimensional picture, it suffices to solve the corresponding transport equations along different streamlines within the object.

The other reason is that, in my opinion, the use of complex two- or three-dimensional problems complicates the simulations and specially the data preparation, but does not add reliability to the simulation results, since involves numerous assumptions about two or three dimensional structure and properties of the simulation objects which cannot be tested. The example from Sect. 4.4 demonstrates that one-dimensional models, more workable and manageable, can compete with two-dimensional ones successfully. However, those who prefer complexity can, likely, apply the method characteristics as well.

Whatever models we use, less or more complex, they are not more than approximations of real objects and processes, always false according to Mesterton-Gibbons (1989), Morton (1993), Beven (2005). However, these approximation models yield practically acceptable results often. Otherwise nobody would use modeling. The suggested approach does not differ from other approaches in this respect. It is not absolute accurate description of the reality. However, as shown in Sect. 10.4, it is able to solve complex enough problems. It does not use fictitious ad hoc parameters like the dispersion coefficient, but only real physical entities like hydraulic dispersion and shares of the total flux carried by streamlines with different velocities which can be evaluated by the use of nonreactive tracers or even reactive if values of their properties responsible for their interaction with surroundings are known. Of course, we cannot evaluate numerically the uncertainty of our simulations in a provable way. However, the suggested approach with its flexibility in fitting factual observations seems to me better and practical than the model which is not sound physically and mathematically and is not able to fit the observed data.

For realization of this approach, it is necessarily that each field experiment of mass transport would include observations on, at least, one nonreactive tracer. It is very important to evaluate the maximal pore velocity as accurately as possible. It means more often sampling of the solution in the very beginning of the solute transport experiments. It is desirable that the sampling was going on as long as the solute concentration stays measurable.

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Chapter 11
Conclusion

Great physicist Nobel Prize Winner Feynman (1965) wrote. "Science is uncertain; the moment you make a proposition about a region of experience that you have not directly seen then you must be uncertain. But we always must make statements about the regions that we have not seen, or whole business is no use". Hydrogeological modeling, as hydrogeology as a whole, is a science. Even more, they are an applied science. Their results are used for practical and often very responsible decision making. Hydrogeologists, including modelers, usually, if not always, "must make statements about the region we have not seen" and make decisions based on incomplete and erroneous data (US EPA 1987). Therefore, the issue of finding effective decisions under condition of uncertainty is one of the most important for them and for the users of the information provided by them.

Contemporary computational technique permits simulating about any predictive problem based on up-to-date hydrogeological theories and concepts. The real issue is reliability of the simulation results, their uncertainty. Geological objects and their properties are not known in full and how the unknown can affect the simulation results is impossible to evaluate. Hornung (1990) writes: "One cannot substitute lack of theory and/or data by sophisticated mathematical models for parameter identification".

Thus, effective decisions, the best possible decisions in some predefined sense, must be the goal. Nevertheless, those decisions are still uncertain and do not warrant success. Even a post audit demonstrating failure or success of a decision does not mean that the decision was bad, or good. In 1960s or 1970s I have, read a book by an American author, I guess the author is H. A. Simon, about decision making. One of his examples impressed me strongly. A person who needs to come to New York from San Francisco asks his friend whether it is better to fly or to go by car or train. The friend advises to fly. The person flies. The airplane crashes. The person perishes. Thus, the post audit is disastrous, but does this mean that the advice and the decision to fly were bad? The successful post audit does not make the corresponding decision good either. Possibly, the same result could be achieved in more effective economically or technologically ways. Thus, we must judge the quality of decisions, considering only the information available at the time of the decision making.

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In my opinion, the engineering experience, where it exists, seems to be the best practical tool for estimating probabilities of failures. For example, construction of typical family houses in typical and well studied geological conditions makes geotechnical explorations unnecessary often. Construction of small dams and reservoirs might be also based on simplified or reduced explorations. Practitioners know what models and model parameters are best for evaluating the dam stability and the losses of water from the reservoirs in given geological conditions. They may be wrong sometimes, and the rate of the failed decisions can be interpreted as an approximation of the uncertainty.

However, what if the required experience does not exist? This happens usually in with unique projects which failures can cause great financial or environmental loses. This book suggests one of possible approaches to how "to do the best" in such situations. The contemporary computers and computational techniques permit developing a surrogate of the engineering experience, applying simulation model or models based on geological considerations to more complex models with fully known properties, called real worlds. (The certainly known details of actual objects can and must be included in the real worlds). Comparing the results obtained by a simulation model (or models) applied to numerous real worlds with different properties and their distributions permits evaluating how different factors could affect the simulation results for a given predictive problem. This is what I call the two level-modeling. Essentially it is the Monte Carlo simulation only the other way around: the real worlds are changing, but the predictive model remains the same only its effective parameters are different for different real words as demonstrated by the conceptual examples in Chaps. 5–8.

Since the factors affecting the 'observations' in the real worlds are numerous and not all of them are taking into consideration in the simulation model or models, the issue arises how to generalize the results of model calibrations on different real worlds in a practical, workable, way. The transforming mechanisms, describing how the actual geological parameters convert into effective parameters of the simulation model in the accepted formulation of the predictive problem, can be one way of such generalization. The transforming mechanisms discussed in Chaps. 6–8 demonstrate clearly that in the case of dynamic processes such as underground water flow and mass transport the converting of actual properties into effective parameters is not of a statistical nature. The effective parameters are characteristics of the systems made up by impacts, geological conditions, structures of models, boundary conditions, criteria of effectiveness, monitoring networks and time. The transforming mechanisms provide the effective parameters only for the systems in which they are obtained. Any changes within the systems lead to changes of their transforming mechanisms. Thus, the transforming mechanisms and parameters effective for predicting water table or hydraulic heads may not be effective for evaluating streamlines or fluxes or solute transport.

The transforming mechanisms, in particular their affecting factors, can be a tool for developing the methodology of field investigations. They demonstrate how important is the knowledge about geological properties of different parts of the object for the accepted formulation of the predictive problem. They can be applied

to formulate and solve inverse problems or, more accurately, to find actual parameters of more sophisticated models (objects) applying less complex interpretation models (Chap. 9). The suggested approach is similar to the approach to interpreting geophysical data and in particular to the data of the electric prospecting. And often the correctness or incorrectness of a given formulation of an inverse problem can be evaluated prior to starting field explorations.

It should be emphasized once more that the transforming mechanisms and two-level modeling do not eliminate the uncertainty of the simulation result. I do not insist also that the suggested approach is the only possible or the best for alleviating the issue of the uncertainty of hydrogeological simulation results. I hope that this work can help in search of other, may be quite different, ways to making hydrogeological modeling more informed and consequently better.

In this edition of the book, a new chapter, Chap. 10, is included. It is devoted to solute transport through porous media. The classical convective–dispersive model of the solute transport is that rare case when the model recognized by scientific community does not do the job it is supposed to do. The cause of this is two governing parameters of the classical model. One of them is the mean pore velocity which excludes from simulation hydrodynamic dispersion, the main factor affecting solute transport when the convective transport exceeds the diffusion process considerably (US EPA 1987). The second is the dispersion coefficient, a fictitious parameter which, as if, compensates for exclusion of hydrodynamic dispersion, but how it does this job was never explained. The method suggested in Chap. 10 is based on advective solute transport equations including hydrodynamic dispersion directly. The method reduces the solute transport model to solving partial differential equations of the first order and is very flexible. The ways of evaluating hydrodynamic dispersion are suggested also.

Hydrogeological modeling is a science only in part. Its considerable component is art requiring imagination and boldness. And if a scientific method in hydrogeological modeling exists, it "*is nothing more than doing one's damnedest with one's mind, no holds barred*," as the other Noble Prize Winner (Bridgman 1955) wrote. He likely meant physics, but I believe, this is true for hydrogeological modeling as well.

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Afterword

Before coming to the United States in 1991, I worked for 35 years in applied geophysics, hydrogeology, geological engineering, and as a professor at two Universities in the Soviet Union. In this country I work for 20 years: with a private firm on projects of Environmental Protection Agency (U.S. E.P.A.), as an instructor in a few colleges, a developer of models of underground flow and mass transport in the University of Georgia, where I received a Master Degree in Applied Mathematics, and as a grantee with U.S. E.P.A. I think that comparison of my Soviet and American experiences may be of interest for readers.

In the very beginning of my professional carrier, I tried to apply statistical methods as much as I could to the data obtained by my colleagues and me. My colleagues were appreciative when I used such statistical methods as regression analysis, analysis of variances, discriminant analysis and some others to their data especially when the data sets were huge. The methods made their reports look more considerable and scientific. But they were usually skeptic about confident intervals and probabilities related to hypothesis testing, regressions and so on. Their skepticism, based on their practical experience and common sense, made me reflect on the role of the statistical methods in geological applications. The results of my reflections are presented in Chap. 3. Briefly, although statistics is an effective tool for analysis of geological information, it is useless for the provable evaluating the uncertainty of simulation results in the case of modeling dynamic processes. In 1974, I wrote a pamphlet (Gorokhovski 1977) in which I discussed this issue. Many colleagues were positive about my work in personal communications. But a couple of well known geologists stopped speaking to me for pretty long time. However, no positive or negative reviews appeared in professional publications. An American publisher bought the right to publish the pamphlet and I got my first five hundreds American dollars. This made my wife Inna happy: she could shop in 'Berjozka', where only people having foreign currency could shop, the privilege not available to most Soviet citizens. But the pamphlet was never published abroad.

At that time I have already been aware of the philosophical concept that all models are false and therefore it is impossible to prove the validity of modeling. But we can reiterate about the uncertainty of the simulation results as much as we wish. The models remain our tool, likely our best one, for envisioning the effects

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induced by natural or man made impacts on geological surroundings. So in my opinion, the goal should be finding how to achieve the best with what we have, as US EPA (1987) states.

Once, while preparing simple problems for my students on evaluating effective hydraulic conductivities, like those presented in Sect. 6.2, I found that some of the effective hydraulic conductivities obtained by the least squares method are negative. It was not the first time that I obtained physically incorrect effective parameters. Following to the common practice, I discarded those results as incorrect based on the definition of incorrectness. However, formally the definition assumes the absence of a mathematical solution. The examples were so simple that they permitted obtaining analytical solutions. Thus, solutions exist, were unique and stable. Nevertheless some of the solutions had physical meaning, being positive, and some did not. Thus, the issue could not be related to the model identification problem formulation. Then what was this? Two weeks of jogging and thinking led me to the concept described in Chap. 5.

I was happy with my finding, in particular with the properties of the affecting factors. However my concept of the transforming mechanisms and their properties seemed so self-evident that I was concerned that somebody else would come to it soon inevitably. To keep my priority, I wrote a paper (Gorokhovski 1982) and sent it in a paper repository. Such repositories in the Soviet Union did not require independent peer reviews and provided a very fast registration of the received material as a paper (3 months). Then the paper could be referred to as a publication. (It could be ordered and bought also.) Later the concept was published two more times (Gorokhovski 1986, 1991).

To my knowledge, the concept was original. Since it contradicted to the common notion, existing at present even, that the effective parameters of hydrogeological models are some statistics of the pertinent property values, the examples in my publications were such that they could be easily checked using a calculator or even by hand. But again, my colleagues demonstrated little interest to the concept. No response, positive or negative, appeared in professional media, though in personal communications they called it interesting and promising. (Sorry, I am not accurate. I had one negative response. A prominent Soviet hydrogeologist after reading my first paper on the transforming mechanism, Gorokhovski (1982) told me: “You are not modest”, and that was it. The reason for such severe judgment was the phrase ending Chap. 5 about the possibility of using the transforming mechanisms not only in hydrogeology but in other fields as well.) So I decided that there was a need for a detailed publication with more examples, maybe slightly more sophisticated, but transparent still.

At that time I worked as an associate professor of the Geology and Geography Department of the Rostov State University. My teaching load in the Spring semester of 1991 was 16 class hours a week, plus 10 course projects, plus 13 master thesis, plus consulting. (I mention only my last semester with the University, because I remember it distinctly. But that load was close to average, if to exclude master theses which we did not have in the winter semesters.) My desk was one of five in a shared office. A typewriter occupied the sixth one. We

consulted students and performed all necessary jobs in this office. For a short time, a real PC was available to me but only two hours per week. I was deprived even those hours very soon. Instead I got, in my full possession, a Soviet PC. The PC had a RAM of 64 Kb and a tape recorder instead of a hard drive. My graduate students used this PC for solving some simple problems related to their theses. I used it for preparing my lectures and other materials and for solving some problems related to teaching. In other words, there was no hope for me to develop my concept further in those circumstances.

In 1990 I met and befriended Dr. Zia Hosseinipour, an American scientist working on a project of cleaning up the low flow of the river Don. Returning to the United States, he asked me whether I would like to work there. My response was immediate: "Yes." For me as for most Soviet scientists working in the United States was a dream. The American science, scientists and work conditions, including salaries, were a benchmark. I hoped also that I would be able to continue my work on the concept of the transforming mechanisms and some other projects.

In the spring, 1991, I got an invitation from an American firm to work on a project. To have an invitation for a job abroad was not enough for leaving the Soviet Union at that time. You needed your bosses' consent. My University bosses did not want me to go. To make a long story short, being in complete despair, I took the liberty calling to Professor V. I. Sedletski. We were not friends. He was a head of the Mineralogy Chair of the department. More essential, he was a vice-president of the North Caucasus Science Center of Higher School. He told me that he needed a couple of days. Then I should start the process again. I got the desired permission to leave for the United States four days later. I owe the deepest gratitude to V. I. Sedletski still.

About 2 months later Zia Hosseinipour introduced me to Dr. James Martin, Head of the Athens, Georgia, branch of the company that hired me. Dr. Martin immediately took me to my office. My first American shock happened when I had seen it: two desks, one with PC and the other with telephone and a chair to travel between the desks. The office was mine only!

I started working, and nobody asked what I was doing during the first 3 months. It was absolutely different from my previous experience. In the Soviet Union, every supervisor asked you how your work was going, whether it was going accordingly to the planned schedule, and so on. And most annoyingly, it did not matter whether the supervisor understood or not what you were doing, the supervisor told you what to do and how to do it. So I was a little worried that Dr. Martin did not ask, teach and give advices to me. Zia explained that James considered me as an expert in my field. When I finally finished my project, he would send it for review. At the time being, if I had a problem, I should go to James and he would do everything he could to help me.

I got a problem when the project was almost finished. James passed me an instruction on conducting the sensitivity analysis. According to the instruction, I had to select the most important model parameters and to evaluate the model's sensitivity to each selected parameter, having fixed all others on their average

levels. In my case, the block of the model describing mass transport through the vadose zone, contained 23 parameters when the zone was assumed homogeneous.

How to decide which parameters are most important and on what average levels the not so important parameters should be fixed were not clear: the task was to validate the model in general without any specificities related to object structures and properties. Even if I selected the important parameters correctly and fixed all others on the right average levels, why would the sensitivity of a parameter obtained in such a way be representative? It can depend essentially on combining particular values of entire sets of the governing parameters. As I understand, the requirement or advice to fix all other parameters on their average level was dictated by the desire to make the sensitivity analysis workable. But there are other ways to make the sensitivity analysis workable, at least in my case. The most natural way is to perform the sensitivity analysis in the dimensionless form as I taught my Soviet students to do. My model was governed by three dimensionless parameters in the steady-state version and by four or five ones in the transient version. All these parameters are important. The sensitivity could be studied in the maximal realistic domain comprising all participating parameter values. The results for such a small number of the dimensionless parameters can be presented as contour maps. They can also be recalculated for any set of all actual parameter values. So I came to James and refused to do the sensitive analysis as the instruction required. He asked: "Why?" I explained. And, the second shock, his response was: "Well, do it as you consider the best". In the Soviet Union, my boss would either tell me: "Do not pretend that you are the cleverest one. Do what you are told to do" or, if I were more fortunate, the boss would make me send a detailed letter to the instruction's authors and wait for their response.

I could say more positive words about the conditions under which scientific researches are being done in the United States. Sure there is control. But this is not a control by the administration usually but by peers. They review your project, its implementation on different stages and the final product. And you can dispute their conclusions if you disagree. The administration helps you, since you do the job. (They are for you, not you for them.) They also help you to get any information you wish. (I found here the Russian text books on mathematics which had been used in Russian schools more than sixty or even seventy years ago. I could not find them in the Soviet Union.)

However, not all my impressions related to scientific research in the U.S.A. are so positive. I have been surprised by the standard approaches to the applied scientific researches by many of my American colleagues. The above instruction on the sensitivity analysis is just one example. It describes a standard procedure which does not take in consideration the specificity of the situation. The standards are useful and convenient. They save time and serve as a safeguard for engineers. But they do not have any relation to the real science and scientific research. Geological explorations deal with objects which are not known in full. In this sense they are scientific, and the best way to conduct them is "doing one's damnedest with one's mind" (Bridgman 1955). I taught my Soviet students that if they act as engineers, they have to follow standards to protect themselves, even if

they do not like or disagree with the standards. But if they work as researchers or scientists, the only limitation on their work is the detailed protocol of their actions and clear presentation of their concepts and results. I rarely observed my American colleagues, realizing such a scientific approach, though the protocol for them seems to be about a holy thing.

Soviet hydrogeological models had bad interfaces in my time. This required that their users understood well hydrogeological structure and properties of the object as well as the process they were simulating and its computational algorithm. They must be prepared to make non-trivial decisions sometimes. On the other hand, the American models are user friendly: their developers try to foresee and prevent any issue that a user could meet. And this is very convenient and effective, if the modeler is a professional. However, the convenience permits performing modeling by lay-modelers as well. The first American model, I worked with, led you through simulations, prompting what to do and even gave optional model parameters values if you had issues with their assigning. Once a colleague, who had a master degree in the environmental protection and worked with the same model, asked me to explain what the hydraulic conductivity is. In turn I was interested to know how she simulated her problems, having no notion on the hydraulic conductivity. She explained that she just followed prompts of the software while assigning different properties to different soils. I think that the example does not require any comment about the uncertainty of simulation results.

The above example leads me to comparing the Soviet and American education systems. When we just came to the United States, our American friend who was teaching mathematics and Russian in a high school invited my wife to visit a lesson on mathematics in his freshman year class. When I met my wife that evening, she was excited: the lesson started with repeating the table of multiplication. In the Soviet Union, we had to learn it by heart in elementary school and never returned to it again. I even cannot imagine a student of the fifth grade not knowing the multiplication table in the Soviet Union.

I taught precalculus in several colleges in this country. There was no such subject in Soviet Universities and Institutes in my time. All Soviet students were studying the same subjects and in the same details. (Those who wanted to get some additional knowledge usually had the opportunity to do this.) The students entering the Universities and Institutes that required knowledge of algebra, geometry and trigonometry had to pass entry tests. If they were not prepared properly, they failed.

The students in geology, hydrogeology, geological engineering and geophysics of all Universities had the same syllabi. (Again, those who wanted to get some additional knowledge usually had the opportunity to do this.) Any future geophysicist studied general geology and hydrogeology, paleontology, historical geology, mineralogy, tectonics, geology of the Soviet Union and so on, though in less detailed comparing to geologists and hydrogeologists, besides geophysics and pertinent physics and mathematics. So it was expected that geophysicists were aware of hydraulic conductivity, geological age, and most other main geological notions and geologists and hydrogeologists have the knowledge on geophysics

which permits understanding of methodology and interpretation of geophysical explorations. Such education makes easier teamwork and even changing the fields of interest as it happened to me.

When I met my first American colleague in his University office, he was on the phone, explaining somebody the method of characteristics. This was also some kind of surprise. I knew just a few Soviet hydrogeologists who were able to explain the method of characteristics: maybe, half dozen not more. And here the first one met knew. I was delighted. But later I came to the understanding that many American hydrogeologists are rather mathematicians applying mathematics to hydrogeology. Hydrogeology seems secondary for them, just a field for the applied mathematics.

Returning to my first American model, it was defined as a screening level one and not interesting *per se*. It comprised two blocks. The first one simulated the one dimensional mass transport from a landfill through the vadose zone which could be piece-wise homogeneous. The second block simulated filtration within a homogeneous confined aquifer on the horizontal base. The flow in the aquifer was considered one-dimensional and steady-state with constant and known seepage. No sorption, no degradation. The goal was to evaluate the arrival time for the contaminant from the landfill to an intake well which also worked in a steady-state regime.

I was interested in the first block mostly. The block simulates input of the pollution in the confined aquifer which seems to me a little strange. Sensitivity analysis of the simulation results showed that for some physically acceptable values of the dimensionless parameters and the pertinent physical characteristics the contaminant mass coming into the confined aquifer were negative. Before writing my report, I advised the leader of the team working on the model developing about my discovery. He did not show any surprise and told that this problem was not major and would be corrected. I guess that he knew already about the problem.

I mention this story not to demonstrate that American modelers are bad. Contrary, they are thorough professionals. Although the model I worked had been in practical applications already, it was in a stage of development still, so errors could happen. The reason for me to tell this story came later when I was presenting my dimensionless sensitivity analysis on a conference. I concluded my presentation by saying that I discovered the negative concentration in the output of one block. We cannot expect that a modeler solving a practical problem has time and possibly skills for performing such thorough analysis. I suggested that every model which is to be used in practical applications must be tested and licensed by an independent body. The response of the audience was instant and unanimous: “No, this is not the American way”. My arguments that they go to licensed doctors and lawyers, send their kids to licensed schools and so on did not change the response of the colleagues: licensing the models developed by them is not the American way.

Let us return to my concept of the transforming mechanisms and two-level modeling. In 1993, I told a known American geostatistician that effective

parameters of hydrogeological simulation models are not statistics and explained why. He answered that it was very interesting and that he liked my approach. Later I sent him my paper (Gorokhovski 1996). His response was brief: "I like this less". I never heard from him again. I gave my paper to another well known geostatistician during the same conference. He promised to review the paper and to send his review to me. He did not. I asked him about his opinion on my paper when we met in at another conference. He told me that he read it in airplane on his way back from the previous conference, was very interested and going to send me a review but could not find my paper. He asked to give him one more copy. I sent it immediately. I never heard from him again. I tried to publish several papers on my concept and made several presentations in the United States. Some my papers were rejected. (Interestingly, one review started with phrase: "I do not understand what the author is about". Well, if you do not understand, it would be reasonable to return the paper to the editor. But the reviewer continued with unmerciful critique of what he or she did not understand. When I asked the editor to pay attention to this fact, he responded that he trusted his reviewers.) Any way, a couple of papers and texts of my presentations were published. The response was the same as in the Soviet Union: no response. My conclusion was also the same: I have to describe the concept in a more detailed and still transparent form. To do this has taken a long time and arduous effort which I do not want to describe here. But if you read these lines, then I have fulfilled my goal. It would not be possible in Russia, and I am grateful to the United States of America for giving me this wonderful opportunity,

P.S. to the second edition:

In several lines above, I criticize an American reviewer of my first attempt to publish a paper in U.S. My recent experience shows that the issue is not a country but rather reviewers and editors themselves. Working on Chap. 10, of this edition, I decided to publish a part of it related to the suggestion to reject convective-dispersion model and to include hydraulic dispersion in solute transport simulation process directly, i.e., to consider only advective transport under different actual pore water velocity and to sum properly the results obtained for different velocities, in a respected European hydrogeological journal. The paper was rejected. The reviewers recognize existence of the issue with simulation of the long tails of the observed long tails of breakthrough curves but hold that it can be resolved by many ways. They do not mention a work stating this fact and ignored the list, long enough, of the works, to which I refer, whose authors concerned with the issue still. One reviewer states: "To derive the velocity distribution and the share of flux from different flow paths from non-reactive tracer transport, it is not acceptable." Why it is not acceptable remains a puzzle. The reviewer ignores my demonstration related to evaluating and usage those velocities. Or: "The hydrodynamic dispersion in the model was accounted by dispersion coefficient". My argument on impossibility to find physical and mathematical description of the mechanisms permitting the dispersion coefficient to compensate for hydraulic dispersion are just ignore as well as on inconsistence of physical representation of the dispersion

coefficient, and so on. The reviewers and editor do not dispute my physical or mathematical arguments. The reviews are rather statement of the absolute belief in the convective-dispersive model and the fictitious dispersion coefficient which does not require any scientific argumentation.

Somewhere in 1980s, I submitted a paper criticizing existing then approach to assigning effective parameters to hydrogeological simulation models in a Soviet journal. Once, being in Moscow, I met one of the reviewers of the paper who told me that his review of my paper was positive. Since I heard nothing from the journal, I met its editor. The editor told me that they would not publish my paper, since their goal was promoting the method I criticized. "What about the positive review?" I asked. The answer was: "You are a mature man. You should know that there is no problem for us to get as many negative reviews as we want". We parted peacefully and the paper was never published. However, I like more the approach of the Soviet editor than the letter from the editor from the European journal: "We are sorry that your submission was not successful this time. We do appreciate your interest in publishing in HJ and hope that you will consider doing so again in the near future".

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