

# Preface

The subject of this monograph lies in the joint areas of applied mathematics and hydrogeology. The goals are to introduce various mathematical techniques and ideas to applied scientists while at the same time to reveal to applied mathematicians an exciting catalog of interesting equations and examples, some of which have not undergone the rigors of mathematical analysis. Of course, there is a danger in a dual endeavor—the applied scientist may feel the mathematical models lack physical depth and the mathematician may think the mathematics is trivial. However, mathematical modeling has established itself firmly as a tool that can not only lead to greater understanding of the science, but can also be a catalyst for the advancement of science. I hope the presentation, written in the spirit of mathematical modeling, has a balance that bridges these two areas and spawns some cross-fertilization.

Notwithstanding, the reader should fully understand the idea of a mathematical model. In the world of reality we are often faced with describing and predicting the results of experiments. A mathematical model is a set of equations that encapsulates reality; it is a caricature of the real physical system that aids in our understanding of real phenomena. A good model extracts the essential features of the problem and lays out, in a simple manner, those processes and interactions that are important. By design, mathematical models should have predictive capability. In this monograph we develop transport models in hydrogeology. Obviously, subsurface phenomena are highly variable and many mechanisms superimpose to give what we observe. Our models do not always try to include every mechanism. We may try, for example, to study only diffusion and adsorption in an effort to understand the interactions between those two processes; in doing so, we may ignore other mechanisms. Therefore, the philosophy of modeling is much different from writing down equations that include every possible effect, with a plethora of parameters, and then using a computer or software package to obtain solutions numerically.

In this monograph a mathematical model generally means a set of partial differential equations (PDEs) that simply describes a physical problem. The equations are typically parabolic or hyperbolic evolution equations. The equations arise from mass balance and relate diffusive-dispersive, advective, and reactive processes involving chemical reactions. Hydrogeologically, the monograph is less about the kinematics and dynamics of groundwater flow, and more about the transport and reaction of solutes in the groundwater. There are a

large number of problems examined in detail; some of these involve more advanced mathematical techniques than one usually encounters in hydrogeological treatments, and more attention is paid to the mathematical issues. In this sense the monograph leans toward the mathematics side. Therefore, this monograph is not a systematic development of the theory of transport processes, but rather a compendium of various simple models that help us understand such processes.

The prerequisites are not extensive. No knowledge of the geosciences is required—just a good physical sense and a willingness to think about physical concepts. Although not absolutely necessary, some knowledge of PDEs will be helpful, particularly PDEs associated with elementary fluid dynamics. In later portions of the monograph some knowledge of phase plane analysis is beneficial. A student who has studied post-calculus differential equations and has read an elementary PDE text can read most parts of the text.

Understanding diffusion processes is fundamental in hydrogeology, both for dispersion of solutes and for the evolution of the head. Therefore, the book begins in Chapter 1 with a review of some of the main ideas associated with the classical diffusion, or heat, equation. These ideas include techniques for solution of the diffusion equation on both bounded and unbounded domains with a variety of boundary conditions. The behavior of solutions is discussed, including the maximum principle. Those familiar with elementary ideas in PDEs could skip this chapter.

Chapter 2 contains the core material on the transport of solutes through porous media—their dispersion, advection, and adsorption. Many examples, which form the basis of the remainder of the monograph, are worked out in detail. Techniques include eigenfunction expansions, Fourier and Laplace transformations, perturbation methods, asymptotic analysis, similarity methods, and energy methods. I have started with this material, usually involving one-dimensional flows, rather than first covering the standard notions of hydraulics and flow patterns, which are examined in Chapter 5. With this approach, the student can appreciate right away the variety of modern environmental problems involving the transport of contaminants without having to first wade through the geometries of well location or other issues concerned with the form of subsurface velocity fields.

In Chapter 3 we discuss special types of solutions called traveling waves. These types of solutions and their stability are greatly beneficial in understanding how different physical processes interact during the evolution of the flow. The predominance of these types of solutions throughout the monograph reflects the author's own interest in them, as well as their prominence in the literature.

Chapter 4 introduces some of the ideas of filtration theory, where particles get sieved out from the medium. There is a discussion of the Herzig–Leclerc–LeGoff model as well as some refinements. The key development is the modeling of processes where the porosity is not constant.

Patterns of flow are discussed in Chapter 5. This is a standard chapter that addresses issues associated with the mechanisms that produce velocity fields and transport. Thus, we discuss Darcy's law, the Dupuis approximation, unsaturated media, and the modeling of flow fields near extraction wells. This material

is very classical and can be found in any hydrogeology book. Certainly, a logical step would have been to place this material at the beginning of monograph. However, the goal was to put emphasis on some of the concepts and models in solute transport, a subject of intense environmental interest, rather than first develop the classical subject of ground water flow.

Flow through porous rocks involves many interesting phenomena relating to porosity-mineralogy changes. Chapter 6 develops some simple models useful in understanding these process. There we study both the propagation of traveling wave fronts on unbounded domains and numerical models on finite domains. The material here can serve as a lead-in to an advanced treatment like P. Ortoleva's *Geochemical Self-Organization*, where pattern formation is discussed in detail.

There are several exercises interspersed throughout the book rather than collected at the end of sections. These are meant to extend or illustrate ideas, or verify facts stated in the exposition, rather than reinforce concepts, as would be the case in an elementary textbook.

Over one hundred references are collected at the end of the book. There has not been an attempt to provide a complete bibliography, and thus many references, especially research articles, have not been included. However, the references listed should provide the reader with a stepping stone to a thorough literature search. There are a few references listed that are not cited directly in the text.

Finally, concerning notation, hydrogeology is a subject practiced by geologists, civil engineers, applied mathematicians, and others. As a result there is not a totally standard notation used in all areas. Porosity, for example, is denoted by  $n$ ,  $\theta$ , or  $\omega$ , depending upon the source. To make adjustments easier, there is included a list of symbols in the appendix. The appendix also includes brief sections on the numerical solution of partial differential equations with programs in MATLAB and Maple. The numerical inversion of Laplace transforms is also included.

My own introduction to mathematical hydrogeology began about a decade ago, and I owe my colleagues and students a great acknowledgment for their patience in listening to my seminar talks and courses on hydrogeology, and for sharing their knowledge with me. This monograph grew out of those seminars and courses. Special thanks go to Professors Steven Cohn, Glenn Ledder, and Tom Shores of the Mathematics and Statistics Department at UNL, Professor Vitaly Zlotnik of the Geosciences Department, and Professor Michelle Homp, a former student, now at Concordia University. Bill Wolesensky, a current Ph.D. student, has read a lot of the manuscript and made many important observations leading to clarity and correctness. During most of the writing I was supported by the National Science Foundation on grant DMS 9708421. The University of Nebraska Research Council also generously supported the efforts, as well as the College of Arts and Sciences through a one-semester sabbatical.



<http://www.springer.com/978-0-387-95276-5>

Transport Modeling in Hydrogeochemical Systems

Logan, J.D.

2001, XIV, 226 p., Hardcover

ISBN: 978-0-387-95276-5