Introduction to Environmental Modeling

The textbook presents an understanding of how basic physical descriptions can be translated into mathematical analogues that provide an opportunity to investigate environmental processes. Examples come from a range of hydrologic, atmospheric, and geophysical modeling problems. The emphasis is on simple examples and calculations that add to understanding. The book provides a sense for the meaning of mathematical expressions, a physical feel for their relations to the processes that they describe, and confidence in working with mathematical solutions.

Addressing environmental modeling problems from a scientific basis requires integration of physical understanding, mathematical skill, courage in making reasonable approximations, and transparency in identifying strengths, weaknesses, applicability, and limitations of the models formulated, employed, and solved. From this perspective, embarking on environmental modeling requires a student to depart from the familiar comforts of well-defined problems for which there is a well-defined solution. Students need to learn how to tackle often incompletely-defined environmental problems in an effort to understand the unknown elements of the past, present, or future and to learn where further studies are needed to increase understanding. The need to approximate, to span mathematics, science, and computational methods, to critique all elements of an analysis, and to admit limitations on what has been accomplished, all contribute to making environmental modeling an exciting, yet sometimes uncomfortable, activity. The goal of this book, in essence, is to present the timeless basic physical and mathematical principles and philosophy of environmental modeling, often to students who need to be taught how to think in a different way than they would for the average more narrowly-defined engineering or physics problem. Minimum prerequisites for the student reader (for any realistic modeling) include a knowledge of calculus through differential equations, but the book provides the mathematical and physical tools needed as the occasion arises.

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Introduction to Environmental Modeling

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> To the next generation of modelers, Charlotte, Ben, Lucy, Gray, and Iris; and to those who gave them life, love them, and nurture their environment.

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The possibility of using a computer to predict the physical, chemical, and biological responses of environmental systems is an exciting notion that attracts student interest. The elements and processes of environmental modeling, however, are in many ways foreign to the kind of thinking that young investigators exercise during their educational experience. Modeling is inexact, requires physical insight, makes use of mathematics that expresses physical concepts, and is subject to revision and continuing study in light of data and observed system behavior. In developing their scientific background, students often see solving problems of physics as grabbing the right equation for the job. Solution of mathematical equations likewise involves identifying and applying the right techniques. Mathematics and physics books for undergraduates only present problems that are fully specified, can be solved, and that have a single answer. Many of those answers are given in the back of the book. Thus work on a problem is reduced to shooting for a known target solution or at least finding the direct path to the only possible answer. Environmental questions, on the other hand, involve problems that an investigator must define in terms of their component elements to find answers that were previously unknown. Formulation of equations requires information about time and spatial scales. Information that would make even simple models solvable is often lacking. The absence of an a priori answer requires that the modeler not only propose a model and its results but also be the harshest critic of the inadequacies of the model. This dual role requires that the modeler be well versed in fundamental processes and in how descriptions of those fundamental processes can be applied to particular environmental problems of interest. Learning to do this requires much more than a semester or a single book of exposure; it requires experience, success, failure, time, insight, and patience.

This book is intended to provide an introduction to environmental modeling; it is not a book that transforms an individual into an environmental modeler. Those who work through this material, appreciate the thought processes, gain some grasp of the principles involved, and develop fundamental understanding will have been introduced to environmental modeling. Hopefully, they will appreciate the hard work that lies ahead to be able to model environmental systems. The references provided are typically more advanced than the material in this book, with the thought being that the introduction here is adequate to provide an entrée into the more specialized and advanced information. This book, although a modeling book, does not make the leap to implementing either new or existing computer codes. Using codes to obtain collections of numbers and attractive graphics can be hazardous without understanding the principles incorporated into the code, the limitations of the code, the meaning and limitations of the numbers calculated, and ways to make a code

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particularly adapted to a setting of interest. Such activity should only be undertaken after forewarning and gaining an appreciation for the fact that the ability to hit the enter key such that a code executes to expected completion is a minute part of successful modeling. Exercising available codes to good effect is not an introductory element of environmental modeling, and writing new codes is also a process that often requires advanced computer science skills.

This book covers the thought processes for modeling, as well as some of the fundamental principles that enable one to model physical processes from a mechanistic perspective. Chapter 1 presents the perspective that modeling requires thinking rather than rote repetition of information. Chapter 2 supports the idea that data alone does not describe a system, but data in light of the context in which the data is collected can describe a system. Chapter 3 encourages examination of data to answer a question in light of a framework, but cautions that the examination is almost never exact so that sources of error must be appreciated and controlled. Chapter 4 stresses the importance of length and time scales in formulating a description of a problem of interest. An overview of the mechanisms that must be operative for a system to undergo change is presented. The mechanisms in this chapter are subsequently incorporated into statements of how systems change. Chapter 6 on dimensional analysis points to the importance of dimensional homogeneity in equation formulation and also illustrates the use of the Buckingham Pi theorem to aid in efficient description of system behavior.

Because algebraic, discrete differences or changes are intuitively easier to understand than differential changes, Chapter 7 formulates some discrete models and discusses their solution. In addition, the effects of numerical instability in solving the equations are demonstrated. Mathematically, Chapter 8 is a review of elements of calculus that a student should have encountered previously. However, the material is presented from the perspective of the relations being physical as well as mathematical statements. This approach is continued in Chapter 9 where integral theorems are introduced that enable equation forms to be rearranged and, in particular, facilitate the transition of the statement of an equation for a finite-sized volume to one that is infinitesimal. Chapters 10 through 13 develop the conservation equations for mass, chemical species, momentum, and energy as the fundamental principles that describe how systems must behave. Both point and integral forms of these equations are encountered. In Chapter 14, approaches are employed for modeling a system in a reduced number of spatial coordinates. As introduced in calculus courses, not considering variability in a coordinate direction usually is achieved by dropping the derivatives in that direction. Here, we emphasize that to ensure conservation properties are honored, variation in a coordinate direction is accomplished by integration over that coordinate. Included in this chapter are the shallow-water equations and the St. Venant equations for channel flow. In Chapter 15, we develop equations that are employed in modeling of porous media. The prime intent is to show that the relevant equations are based on the fundamental conservation principles formulated at a different scale. At this point, equations have been developed for a wide array of systems. Chapter 16 introduces the idea of solving these equations using a numerical method. The presentation is for a simple contaminant transport problem with the objective being to illustrate the thought processes behind

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numerical algorithms that can serve as a springboard to the study of more complex algorithms and processes. Chapter 17 revisits stability considerations for numerical solution of discrete equations. The objective is to illustrate that instabilities, which sometimes seem to be surprising mathematical artifacts, can be thought of as manifestations of improperly operating a system.

In all chapters, questions are inserted within the text and problems are provided at the end of the chapters. The questions are relatively simple and are inserted strategically at places in the text as aids in cementing down processes or concepts just introduced. In a sense, they are speed bumps that encourage a reader to make sure he or she understands what has been written before going on to the next concept. These questions also provide a basis for productive discussions. The problems at the end of the chapter are more comprehensive. They make use of material in the preceding chapter and also integrate material presented previously in the book. The problems do not seek regurgitation of material presented but ask the student to be creative in bringing the material to bear on a specific scenario. Answers to the problems are not necessarily unique; problems may require that some additional information be added so that the problem is completely defined. Work on the problems by groups rather than individuals can be beneficial in some cases, as different perspectives will enrich formulation of problem solutions.

This book is based in part on a course on environmental modeling offered through the Curriculum for the Environment and Ecology (CEE) at the University of North Carolina in Chapel Hill. The authors are grateful to those discerning people who have provided them with insights over the years on modeling and/or on education in general, especially George F. Pinder (University of Vermont), Cass T. Miller (University of North Carolina at Chapel Hill), Randall L. Kolar (University of Oklahoma), Stephen Whitaker (University of California at Davis), Mohamed S. B. H. Ghidaoui (Hong Kong University of Science and Technology), Monica Martinez-Canales (Intel), Herbie Lee (University of California, Santa Cruz), and Robert B. Gramacy (Virginia Tech). The outstanding students who have encountered this material in course offerings have added many insights and much enthusiasm. Their contributions in providing perspective on this material and in confirming its importance to their education has inspired some of the approaches employed here. We are grateful to Gregory Gangi, who encouraged such excellent students to engage with environmental modeling, and to Jaye E. Cable whose educational leadership fostered this course under the CEE umbrella. Two of the students who took the course, Elizabeth C. Christenson and Jillian L. Simmerman, deserve particular mention because their involvement, as well as subsequent contributions as teaching assistants, added greatly to the collaborative atmosphere of the course and to insights into the way material is structured and presented. We thank Matt Lloyd of Cambridge University Press for his unswerving support for this manuscript from the first time it was informally proposed through its completion. We greatly appreciate the efforts of Judith Shaw, who copy-edited the manuscript, and of Caroline Mowatt, who ushered this effort through to publication.

Over the years, many individuals have provided perspectives on the topics of this book through interactions with the authors in professional settings, books and manuscripts, informal conversations, and anonymous writings. Every effort has been made to acknowledge all sources, but the collection of perspectives through the years has resulted in the identity

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of some sources fading from memory while their insights remain. We are grateful indeed to all parties who have informed us on elements of environmental modeling and regret any oversights in explicit recognition. We welcome comments and suggestions involving the use of this book and regret the shortcomings of our presentation.

The first author is ever grateful to and for Genny Gray who has provided generous, unflagging confidence in him throughout the years. Without her participation, the life of the first author would have been incomplete, and the life of the second author would have been impossible. The second author is grateful to Rob McGormley for his encouragement and support during the creation of this work. This collaboration has been a professional and personal activity that both authors recognize as a special privilege.