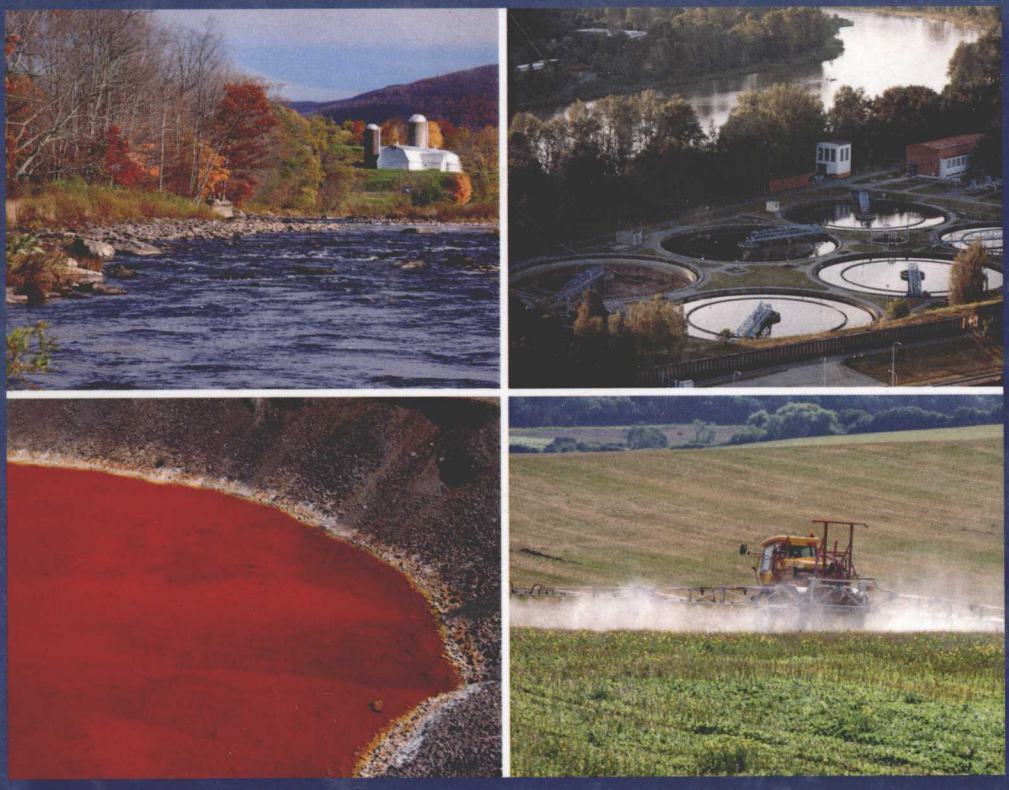
Environmental Process Analysis

Principles and Modeling



HENRY V. MOTT

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Principles and Modeling

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Environmental Process Analysis

To my deceased grandparents, Ida and Floyd Slingsby, and Ragna and Henry Mott;
to my deceased parents, Marge Marie and Henry Valentine, who raised me;
to my sisters, Jean, Judy, and Jane, with whom I shared childhood;
to my children, Harrison, Graeme, and Sarah, with whom I now share adulthood;
to my daughter-in-law, Lana, and my granddaughter, Samantha;
to Marty, my sweet bride, with whom I share a wonderful life.

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Preface

This book is about mathematical and numerical modeling of processes in contexts associated with both natural and engineered environmental systems. In its assembly, I have relied on some very traditional but highly ubiquitous principles from natural and engineering science—chemical equilibria, reaction kinetics, ideal (and nonideal) reactor theory, and mass accounting. As necessary to the contexts of interest, I have incorporated principles from fluid dynamics, soil science, mass transfer, and microbial processes.

Many texts addressing introductory environmental engineering include discussions of these principles, but in opting to semiquantitatively address specific environmental contexts, never really apply them. Introductory modeling efforts seldom tread quantitatively beyond situations that are solved by single, explicit relations. This approach is fully appropriate at the entry level. Broad-based knowledge gained from an introductory course and text is essential to full appreciation of the portability of principles to myriad environmental systems. This text is not intended to replace an introductory environmental engineering textbook but to build on the contextual knowledge gained through completion of an introductory environmental engineering course.

In Chapter 2, some properties of water important to the understanding and employment of chemical equilibria are discussed. In Chapter 3, a collection of the various units describing abundance of components in gas, liquid, and solid systems is assembled. In Chapter 4, several specific conventions of the law of mass action, applicable to specific chemical "systems" are detailed. Then in Chapters 5 and 6, modeling of systems employing Henry's law and acid/base principles is examined. In Chapters 7 and 8, modeling of mixing and reactions in ideal reactors is addressed. These first eight chapters constitute the "basic" portion of this text. These topics and associated modeling work are appropriate for a third- or fourth-year undergraduate

course, beyond the introductory level. I employ MathCAD as a powerful computational tool to illustrate, in the environmental contexts considered, the power of modeling in process analysis. In Chapter 9, I have extended the applications of three nonideal reactor models: completely-mixed flow reactors in series; plug-flow with dispersion; and segregated flow, beyond the level of treatment found in current texts. While containing good "food for thought" at the fourth-year undergraduate level, Chapter 9 is most appropriate for the graduate level.

Traditional water or aquatic chemistry texts introduce and discuss the chemical equilibria of acids/bases, metal complexes, solubility/dissolution, and oxidation/reduction. Mention is made of the proton balance, but this powerful tool is most often discarded or treated cursorily in favor of the seemingly much simpler charge balance. In fact, for systems that are not infinitely dilute (virtually all real systems) the charge balance most often fails at the outset. I have extended the application of the proton balance (or condition) to provide for significant advances in understandings of the acid- and base-neutralizing capacity of aqueous solutions and both solution–vapor and solution–solid systems. I have also demonstrated the relative ease with which nondilute solution principles can be incorporated into chemical equilibrium modeling.

For modeling of systems, traditional texts most often rely heavily upon simplifying assumptions, leading to graphical or approximate solutions, or upon sophisticated chemical equilibrium modeling software for quantitative description of chemical equilibria. Some recent texts have begun to chip away at the computational wall separating pencil/paper/graphical solutions from those involving sophisticated software but have not made significant headway. No other existing text known to me addresses, in transparent detail, the process of coupling mathematics with chemical equilibria and both mass and proton accounting for numerical modeling of chemical equilibrium systems.

Herein, I employ the general mathematical/numerical worksheet software MathCAD to occupy the region beyond approximate solutions and encroaching upon that of sophisticated software. A huge assembly of mathematical capability is available in a "what you see is what you get" user interface. Key to modeling of chemical equilibrium systems is ready capability to write user-defined functions, to program the solution of systems of nonlinear equations, and to create structured-code-like programs, all entirely visible in printable, portable worksheets. In fact, the vast majority of work illustrated in examples of this text has been conveniently exported into the manuscript as captures directly from worksheets. I make few, if any, simplifying assumptions beyond those associated with the first principles used in the mathematical modeling. The modeling efforts described herein, associated with the traditional water chemistry principles, are numerically as capable as those of the sophisticated software but much more flexible. These created models can be used not only to numerically model the equilibria but also to employ the equilibrium modeling to assess the consequences of perturbing the systems. Coupled with Chapters 2–6, Chapters 10–12 constitute the "advanced" portion of this text addressing chemical equilibrium modeling.

Those who will benefit from reading and studying this text are those who wish to mathematically and numerically model environmental processes and systems and who wish to fully understand the connections among the various factors leading to the results. Practitioners, depending upon their level of fundamental understandings, would benefit in a manner similar to students. No specific numerical methods skills are necessary, beyond attention to detail and an understanding that for numerical solution methods to work, they must be started in some vicinity of the final solution, assigning initial guesses to all unknowns sought. Although not absolutely necessary, it is certainly recommended that the reader obtain the MathCAD software and carefully follow through the worked examples. Such an approach promotes both understandings of the principles and mathematical modeling as well as capability for implementation of numeric solutions.

HENRY V. MOTT

Additional MathCAD files that accompany this text are available at booksupport.wiley.com by entering ISBN 9781118115015.

Additionally adopters of the text can obtain the solutions manual to the text by going to the books landing page at www.wiley.com and requesting the solutions manual.

Acknowledgments

I offer my special thanks to four former students, Zane Green, Nathan Kutil, Ulrike Lashley, and Teryl Stacey, who painstakingly reviewed the manuscript of this text, freely offering their time and abilities to make this effort as useful as possible for the students to come. I also offer my thanks to the many graduate and undergraduate students who sat in my classrooms, and with great enthusiasm engaged in the discussions and related efforts necessary to the development of the understandings manifest in the many example problems included in this text. I also offer my heartfelt thanks to my friend and colleague, Melvin Klasi, who, through my many years as a member of the Faculty of the SD School of Mines, was always willing to assist me in my understandings of mathematics and its implementation in modeling efforts.

I also must acknowledge some of my many teachers and mentors. Sam Ruzick and John Willard helped me unlock my love of chemistry, although it was to remain dormant for many of the years I studied to be and called myself a civil engineer. Hank Trangsrud taught me to ask tough questions and then to answer them. Al Wallace was, well, Al Wallace. My good friend Tom Nielsen and I learned much as we tackled the tough problems and topics with which Al charged us. Don Johnstone and Harry Gibbons were instrumental in the development of my understanding of microbes and aquatic insects as living, breathing beings. David Yonge, Erv Hinden, and Ken Hartz helped propel me onward by suggesting, at my MS thesis proposal presentation, that I extend it to a PhD dissertation, although I left Washington State to pursue my PhD. Walt Weber presented me with a challenging and relevant PhD thesis project and solid mentoring and support for its completion. Then, Walt, Don Gray, Linda Abriola, and Rane Curl helped me ensure that my work was top notch. I learned much from my common struggles alongside and interactions with my peer PhD students: Yo Chin, Lynn Katz, Domenic Grasso, Kevin Ohlmstead, Chip Kilduff, Margaret Carter,

and Ed Smith. In the classrooms of Bernie Van Wie, Linda Abriola, Rich Kapuscinski, Jon Bulkley, Rane Curl, Ray Canale, Scott Fogler, and Bob Kadlec, I learned to couple mathematics with physical, chemical, and biological processes. The understandings of the portability of fundamental principles among systems quite naturally arose as an added bonus. In the classrooms of Brice Carnahan and James Wilkes, I learned that quantitative answers need not be exact, but certainly as close as reasonably possible.

I am the primary author of this text; I have no coauthors. However, I have chosen to employ the first person plural, we, in many of the discussions of the text. The knowledge and understandings employed in those discussions and companion examples arise as a consequence of the foundational work I did as assisted and guided by my many teachers and mentors. Their collective pursuit of personal and student betterment certainly contributed greatly to the expertise that I now claim as my own. In this text, when I use the term "we," it is I and my teachers and mentors to whom I refer.

Contents

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Chapter 1

Introductory Remarks

1.1 PERSPECTIVE

From the outset, let us make no mistakes about the purpose and content of this textbook. The main title—*Environmental Process Analysis*—suggests that we will analyze processes. The targeted processes are those operative homogeneously in aqueous solutions, involving the gas–water interface, and involving the water–solid interface. Understandings of the behavior of environmental systems can arise from examination of both natural or engineered processes under equilibrium or near-equilibrium conditions. The effects of perturbations on systems can be determined using the initial and predicted final equilibrium conditions. In addition, understandings can arise from examination of the progress of such processes under transient or near (quasi) steady-state conditions. Then, Environmental Process Analysis is the examination of the processes operative in conjunction with perturbations of environmental systems, either natural or engineered, arising mostly from actions of our society. Certain of these perturbations beget negative consequences associated with actions that, while well-intentioned, contribute to the detriment of an environmental system. Others are intended to positively affect a compromised natural system or to implement a desired outcome within the context of an engineered system. The subtitle—*Principles and Modeling*—suggests that we will employ appropriate principles, develop models in support of our analyses, and employ these models to predict the outcomes from intended or unintended perturbations. Modeling has three distinct levels. Conceptual modeling involves identifying, understanding, and interrelating processes operative

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