# Applied Mathematics and Modeling for Chemical Engineers

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# Preface

The revolution created in 1960 by the publication and widespread adoption of the textbook *Transport Phenomena* by Bird et al. ushered in a new era for chemical engineering. This book has nurtured several generations on the importance of problem formulation by elementary differential balances. Modeling (or idealization) of processes has now become standard operating procedure, but, unfortunately, the sophistication of the modeling exercise has not been matched by textbooks on the solution of such models in quantitative mathematical terms. Moreover, the widespread availability of computer software packages has weakened the generational skills in classical analysis.

The purpose of this book is to attempt to bridge the gap between classical analysis and modern applications. Thus, emphasis is directed in Chapter 1 to the proper representation of a physicochemical situation into correct mathematical language. It is important to recognize that if a problem is incorrectly posed in the first instance, then any solution will do. The thought process of "idealizing," or approximating an actual situation, is now commonly called "modeling." Such models of natural and man-made processes can only be fully accepted if they fit the reality of experiment. We try to give emphasis to this well-known truth by selecting literature examples, which sustain experimental verification.

Following the model building stage, we introduce classical methods in Chapters 2 and 3 for solving ordinary differential equations (ODE), adding new material in Chapter 6 on approximate solution methods, which include perturbation techniques and elementary numerical solutions. This seems altogether appropriate, since most models are approximate in the first instance. Finally, because of the propensity of staged processing in chemical engineering, we introduce analytical methods to deal with important classes of finite-difference equations in Chapter 5.

In Chapters 7 to 12 we deal with numerical solution methods, and partial differential equations (PDE) are presented. Classical techniques, such as combination of variables and separation of variables, are covered in detail. This is followed by Chapter 11 on PDE transform methods, culminating in the generalized Sturm–Liouville transform. This allows sets of PDEs to be solved as handily as algebraic sets. Approximate and numerical methods close out the treatment of PDEs in Chapter 12.

This book is designed for teaching. It meets the needs of a modern undergraduate curriculum, but it can also be used for first year graduate students. The homework problems are ranked by numerical subscript or an asterisk. Thus, subscript 1 denotes mainly computational problems, whereas subscripts 2 and 3 require more synthesis and analysis. Problems with an asterisk are the most difficult and are suited for graduate students. Chapters 1 through 6 comprise a suitable package for a one-semester, junior level course (3 credit hours). Chapters 7 to 12 can be taught as a one-semester course for advanced senior or graduate level students.

Academics find increasingly less time to write textbooks, owing to demands on the research front. RGR is most grateful for the generous support from the faculty of the Technical University of Denmark (Lyngby), notably Aa. Fredenslund and K. Ostergaard, for their efforts in making sabbatical leave there in 1991 so successful, and extends a special note of thanks to M. Michelson for his thoughtful reviews of the manuscript and for critical discussions on the subject matter. He also acknowledges the influence of colleagues at all the universities where he took residence for short and lengthy periods including: University of Calgary, Canada; University of Queensland, Australia; University of Missouri, Columbia; University of Wisconsin, Madison; and of course Louisiana State University, Baton Rouge.

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