Numerical Methods & Modeling for Chemical Engineers

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May 14, 2001

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Numerical Methods and Modeling for Chemical Engineers

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Virginia Polytechnic Institute and State University

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10 9 8 7 6 5 4 3 2 1
To Mary Margaret
This book is an introduction to the quantitative treatment of differential equations that arise from modeling physical phenomena in the area of chemical engineering. It evolved from a set of notes developed for courses taught at Virginia Polytechnic Institute and State University.

An engineer working on a mathematical project is typically not interested in sophisticated theoretical treatments, but rather in the solution of a model and the physical insight that the solution can give. A recent and important tool in regard to this objective is mathematical software—preprogrammed, reliable computer subroutines for solving mathematical problems. Since numerical methods are not infallible, a “black-box” approach of using these subroutines can be dangerous. To utilize software effectively, one must be aware of its capabilities and especially its limitations. This implies that the user must have at least an intuitive understanding of how the software is designed and implemented. Thus, although the subjects covered in this book are the same as in other texts, the treatment is different in that it emphasizes the methods implemented in commercial software. The aim is to provide an understanding of how the subroutines work in order to help the engineer gain maximum benefit from them.

This book outlines numerical techniques for differential equations that either illustrate a computational property of interest or are the underlying methods of a computer software package. The intent is to provide the reader with sufficient background to effectively utilize mathematical software. The reader is assumed to have a basic knowledge of mathematics, and results that require extensive mathematical literacy are stated with proper references. Those who desire to
Preface

delve deeper into a particular subject can then follow the leads given in the references and bibliographies.

Each chapter is provided with examples that further elaborate on the text. Problems at the end of each chapter are aimed at mimicking industrial mathematics projects and, when possible, are extensions of the examples in the text. These problems have been grouped into two classes:

Class 1: Problems that illustrate direct numerical application of the formulas in the text.

Class 2: Problems that should be solved with software of the type described in the text (designated by an asterisk after the problem number).

The level of this book is introductory, although the latest techniques are presented. The book can serve as a text for a senior or first-year graduate level course. At Virginia Polytechnic Institute and State University I have successfully used this material for a two-quarter sequence of first-year graduate courses. In the first quarter ordinary differential equations, Chapter 1 to 3, are covered. The second quarter examines partial differential equations using Chapters 4 and 5.

I gratefully acknowledge the following individuals who have either directly or indirectly contributed to this book: Kenneth Denison, Julio Diaz, Peter Mercure, Kathleen Richter, Peter Rony, Layne Watson, and John Yamanis. I am especially indebted to Graeme Fairweather who read the manuscript and provided many helpful suggestions for its improvement. I also thank the Department of Chemical Engineering at Virginia Polytechnic Institute and State University for its support, and I apologize to the many graduate students who suffered through the early drafts as course texts. Last, and most of all, my sincerest thanks go to Jan Chance for typing the manuscript in her usual flawless form.

I dedicate this book to my wife, who uncomplainingly gave up a portion of her life for its completion.

Mark E. Davis
## Chapter 1

**Initial-Value Problems for Ordinary Differential Equations**  

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