

## Numerical Methods with Chemical Engineering Applications

Designed primarily for undergraduates, but also graduates and practitioners, this textbook integrates numerical methods and programming with applications from chemical engineering. Combining mathematical rigor with an informal writing style, it thoroughly introduces the theory underlying numerical methods, its translation into MATLAB programs, and its use for solving realistic problems. Specific topics covered include accuracy, convergence and numerical stability, as well as stiffness and ill-conditioning. MATLAB codes are developed from scratch, and their implementation is explained in detail, all while assuming limited programming knowledge. All scripts employed are downloadable, and built-in MATLAB functions are discussed and contextualized. Numerous examples and homework problems – from simple questions to extended case studies – accompany the text, allowing students to develop a deep appreciation for the range of real chemical engineering problems that can be solved using numerical methods. This is the ideal resource for a single-semester course on numerical methods, as well as other chemical engineering courses taught over multiple semesters.

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# Numerical Methods with Chemical Engineering Applications

KEVIN D. DORFMAN AND PRODROMOS DAOUTIDIS

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## Preface

Why write yet another book on numerical methods? Having taught this course for a combined 10 years, we have continuously struggled to find a single textbook that works for chemical engineering students. There are outstanding books on the mathematical underpinnings of numerical methods, but the level of sophistication (theory–lemma) is often a turnoff for chemical engineering students and overkill at the introductory stage. There are also excellent generic books on numerical methods that include some engineering applications. We used one such book as a reference for the course, since many students do better with supplemental reading. The challenge with general books is that they do not incorporate sufficient chemical engineering examples, which leads to students wondering exactly how the textbook (which is often expensive) connects to the class. Moreover, with the explosion of online resources, it is quite easy to find explanations of standard numerical methods with the click of a mouse. (Whether those explanations are good or even correct is another issue entirely!) At the other end of the spectrum are chemical engineering textbooks solely devoted to applications with little discussion of the underlying numerical methods. These books provide a wealth of example problems, but they are not suitable for teaching students how to actually solve the problems.

Our goal in writing this textbook is to take a “Goldilocks” approach: not too rigorous, not too applied! At the same time, we want to firmly embed our discussion of numerical methods in the context of chemical engineering applications. The material presented in the book is based on the content of a course in numerical methods developed in our department more than 20 years ago. The book is intended for an undergraduate course in numerical methods, primarily for chemical engineering students. At Minnesota, this is a core course taught in the spring semester of the junior year. The students are taking this course concurrently with (i) Reaction Kinetics and Reactor Design and (ii) Mass Transfer and Separations. This location in the curriculum offers many opportunities to motivate the methods covered in the book and use them to solve realistic chemical engineering problems. For example, we have timed the numerical methods course and the reactors course so that, when we cover systems of ordinary differential equations in numerical methods, the reactors course covers systems of chemical reactions. The students have already taken Transport Phenomena and Thermodynamics in the fall, so these subjects are also covered in the book through examples of problems that could not be solved by hand in the preceding courses.

While we believe this to be the ideal location for the course, we provide sufficient background information for the different problems so that the students can solve them

without necessarily having a previous course in the subject. As a result, the book can certainly be used early in the curriculum, for example in conjunction with Mass and Energy Balances, especially if the goal is to enhance the use of numerical methods in that class and to build a foundation in numerical methods that can be used later in the curriculum. The book would also fit well at the end of the chemical engineering curriculum, when the students have all of the scientific and engineering background but cannot yet solve “real” problems that lack closed-form solutions.

An emerging challenge that we are facing in our curriculum is a lack of programming experience. This is ironic, as it is hard to imagine that students have become any less reliant on computation in their education or their daily life. The problem is that our university (and others elsewhere) no longer requires entering engineering students to take an introductory programming course. Even when such a course is required, it rarely focuses on the aspects that are required for scientific computing. The logic for this evolution in the chemical engineering curriculum is two-fold. The first is commendable, namely creating a manageable course load for students so that they can graduate in a timely manner. Because of the recent expansion of the chemical engineering curriculum in areas such as biology, something needs to be removed to make space. The second is less defensible, namely that students will use packages such as MATLAB or Aspen to solve chemical engineering problems, so they no longer need to be taught basic programming. At a philosophical level, this argument is very troubling – it essentially argues that engineers do not need to understand how their tools work. At a more practical level, although programming environments (such as MATLAB) are prevalent nowadays, they are often used without a solid understanding of the underlying numerical methods. This “black box” approach can easily lead to erroneous analysis and interpretation of results. Knowledge of the underlying numerical methods is essential in order to be able to choose from a suite of options usually available, and use them correctly and efficiently. Numerical methods go hand-in-hand with programming. Moreover, with the discipline moving towards more fundamental, science-oriented research, the students’ background in mathematics is often lacking, and so is their ability to appreciate the power of modern mathematics to provide solutions to cutting-edge problems across science and engineering. Our overall goal in this book is to address this problem with a single-semester, focused course that integrates basic programming skills and numerical methods to solve chemical engineering problems.

## Organization of the Book

The book starts with a review of mathematical problems arising in chemical engineering, highlighting the (restrictive) assumptions which make them amenable to analytical solutions, and thus motivating the need for numerical methods. The problems covered in the rest of the text are (in order): linear algebraic equation systems, nonlinear algebraic equation systems, ordinary differential equation systems – initial value problems, ordinary differential equations – boundary value problems, classes of partial differential equations (initial-boundary and two-dimensional boundary value problems), and

numerical integration. As such, the level of difficulty gradually increases, and the solution methods naturally build on those developed earlier. This arrangement of the material deviates from the standard approach in numerical methods in several substantial respects. For example, we have split up the material on numerical differentiation and integration, which often appear together early in a numerical methods course. The numerical differentiation appears in the context of boundary value problems, where it becomes clear why it is necessary, and the numerical integration is deferred to the end of the book, as its importance in chemical engineering is subordinate to solving nonlinear algebraic equations and differential equations.

For each class of problems, we start with a thorough derivation of the numerical approximation methods covered. We discuss in some length topics such as accuracy, convergence, and numerical stability properties of the derived methods. Topics such as ill-conditioning and stiffness are also covered as they are essential to be able to detect limitations inherent to the nature of the underlying physical/engineering problem we are trying to solve. We devote a separate chapter to dynamical systems, where we also provide an introduction to nonlinear dynamical phenomena.

We show how each numerical method can be programmed within MATLAB. We begin by assuming very limited programming experience, introducing elementary programming concepts in the first chapter. We then build on these ideas as we develop the necessary MATLAB codes from scratch, explaining in a step-by-step fashion their structure, function, and implementation. We then use (and modify) the codes that we built to solve chemical engineering problems. Importantly, this is *not* a book on using canned routines in MATLAB. Rather, we take advantage of MATLAB's easy debugging and interfacing with plot commands to make the course much simpler than would be the case if the students used a structured programming language like C. Indeed, the only canned numerical method that we use in the book is MATLAB's linear solver (the slash operator), and only after we have covered elementary methods for solving linear algebraic systems. We believe this to be a key feature of the book in that we essentially use the MATLAB environment to teach programming. Recognizing that students should also know how to use the canned routines as well, the end of each chapter provides a brief outline of MATLAB's built-in functions, but only after the students have learned the basics. All of the scripts appearing in the book are available as a downloadable resource.

In each chapter, in addition to short illustrative examples, we include detailed case studies that draw from core chemical engineering subjects (mass balances, thermodynamics, transport, kinetics, reactor design). We use these case studies to illustrate the value of numerical methods in solving realistic chemical engineering problems, but also to provide new perspective on problems that students have already seen (e.g. using continuation to generate phase diagrams). These examples are spaced out in such a way so that their frequency increases as the book proceeds. We have found this to be a useful way to organize a course using this book; as the material becomes more difficult, we slow down the pace of new numerical concepts and reinforce their applicability in chemical engineering.

Finally, numerous problems are included at the end of each chapter that address theoretical questions as well as application of the methods to chemical engineering problems. These problems have a wide range of difficulty and depth, ranging from simple short answer problems that test basic concepts to extended questions that we usually assign over several weeks for students to address in teams. A complete solution manual for instructors, including all of the codes required to solve the problems, is also available.

“Dorfman and Daoutidis’s new book is a welcome addition to the undergraduate chemical engineering textbook literature. It provides a very attractive combination of programming, applied mathematics and chemical engineering applications, and is written in an accessible style. The incorporation of example MATLAB codes will be very helpful to students.”

Michael D. Graham, University of Wisconsin-Madison

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