IN THE NAME OF ALLAH,

MOST GRACIOUS, MOST MERCIFUL

INTRODUCTION TO NUMERICAL METHODS WITH APPLICATION TO CHEMICAL ENGINEERING

Emad Ali
AbdelHamid Ajbar
Khalid Alhumaizi
Department of Chemical Engineering
College of Engineering
King Saud Univesity
Riyadh, Saudi Arabia

Academic Publishing and Press, King Saud University
P.O. Box 68953, Riyadh 11537, Saudi Arabia

King Fahd National Library Cataloging-in-Publication Data

Ali, Emad
Introduction to numerical methods with application
to chemical engineering. / Emad Ali; AbdelHamid
Ajbar; Khalid Alhumaizi. - Riyadh, 2008

272 p., 17 x 24 cm
ISBN: 978-9960-55-394-8

1-Chemical engineering
I-AbdelHamid Ajbar (co. author) II-Khalid Alhumaizi (co. author)
III-Title

660.2 dc 1429/6033

Legal Deposit No. 1429/6033
ISBN: 978-9960-55-394-8

This book has been refereed by a specialized committee appointed by the Academic Council of the University. After the reports of the referees, the Council authorized its publication in its 5th session of the academic year 1428/1429 H., which was convened on 21-11-1428 H. (1-12-2007)

Academic Publishing and Press

PREFACE

Many chemical engineering departments in diverse universities around the world, including the one in King Saud University, include in the curriculum a course designed to teach numerical methods applied to chemical engineering. This book is essentially a compilation of the notes the three authors have used to teach this course over the years. We have covered in the textbook the numerical techniques that are most useful to the chemical engineer and that have wide applications. As an introduction to the book, we included a chapter dealing with some practical considerations in numerical methods. The concepts of errors, conditioning of a problem and stability of algorithms were introduced to show the student to what extent he should trust any numerical values obtained by solving a problem in a digital computer. The first type of problems covered by the book is the system of linear algebraic equations (Chapter 2). This choice is in line with the contents of the prerequisite of the course that teaches numerical solutions of mass and energy balance equations. Many linear algebraic equations originate from the applications of steady state mass balance equations. The chapter that follows deals with the solution of non-linear algebraic equations. Chapter 3 is a normal continuation to the previous chapter since many applications of non-linear algebraic equations originate from steady state energy balance equations. Chapters 4 and 5 deal with the solution of ordinary differential equations, initial value problem and boundary value problem, respectively. Students are introduced to numerical solutions of unsteady state mass and energy balance equations as well as to numerical solutions of steady state one dimensional distributed parameter models. The rest of the book (Chapters 6 to 10) deal with the issue of optimization. This issue is divided in three parts. The first part (Chapter 6) deals with linear regression. We choose to start by linear regression (simple and generalized) since it is a subject that has direct applications in other students courses, especially in students labs experiments. Also, the numerical methods for linear regression are essentially those of linear algebraic equations that were covered in Chapter 2. The second part of optimization is divided into three chapters (Chapter 7, 8 and 9). Chapter 7 introduces the students to basic concepts of single variable optimization, and presents some numerical methods. Chapter 8 generalizes the concepts of Chapter 7 to multivariable unconstrained problems. It also provides a number of numerical techniques for these types of problems. Chapter 9 deals with the constrained optimization problems where the Lagrange multipliers method is introduced. The last part of the optimization issue is covered in Chapter 10 where linear programming is taught in detail.

The various numerical methods were presented in the form of flow-chart diagrams. Each numerical method introduced in the text has a solved example associated with it. Virtually, all the examples are chemical engineering problems, spanning wide areas from mass and energy balance equations to kinetics and thermodynamics. The programming language used to teach this book is FORTRAN, and we also rely on IMSL routines. These routines are in many cases sophisticated and are based on special implementation of the basic methods taught in the body of the book. For these reasons, we have introduced at the end of each chapter two sections: a section entitled "Other Solution Techniques". In this section, the students are introduced very briefly to other more elaborate solution techniques, but the objective of this section is also to introduce the students to the special methods and algorithms that are effectively used in the IMSL routines. The second section at the end of the chapter presents some IMSL routines that were commonly used in the teaching of the materials. In addition to all of this, we have presented at the end of the book a collection of FORTRAN programs that can be used directly (without the need for IMSL routines) to solve some basic problems covered in the chapter.

The text is designed primarily for undergraduate students who have knowledge of the fundamentals of chemical engineering and some background in calculus especially linear algebra and differential equations. However, some parts of the book could also be used as part of a first year graduate course on numerical methods. For undergraduate level, the materials that could be used for a 15-week long semester could include:

- Chapter 1: Basic concepts on errors, conditioning and stability.
- Chapter 2: Solution of linear systems. Cuts could be made depending on the materials taught in the prerequisite of the course. For instance, in the chemical engineering department at KSU, a prerequisite course teaches students the fundamentals of Gauss elimination methods. The instructor could focus on LU decomposition and on iterative methods.
- Chapter 3: Non-linear systems. Secant and Müller method could be skipped or assigned as student review.
- Chapter 4: Solution of ODE-initially value problem could be covered in full.
- Chapter 5: Boundary value problem could also be covered in full.
- Chapter 6: Linear regression could be covered in full.
- Chapter 7: Single variable optimization could be covered in full.
- Chapter 8: Multivariable unconstrained optimization, Chapter 9: Multivariable constrained optimization, and Chapter 10: Linear programming are best left to another semester, if available. These chapters could also be taught as part of a first level graduate course.

CONTENTS