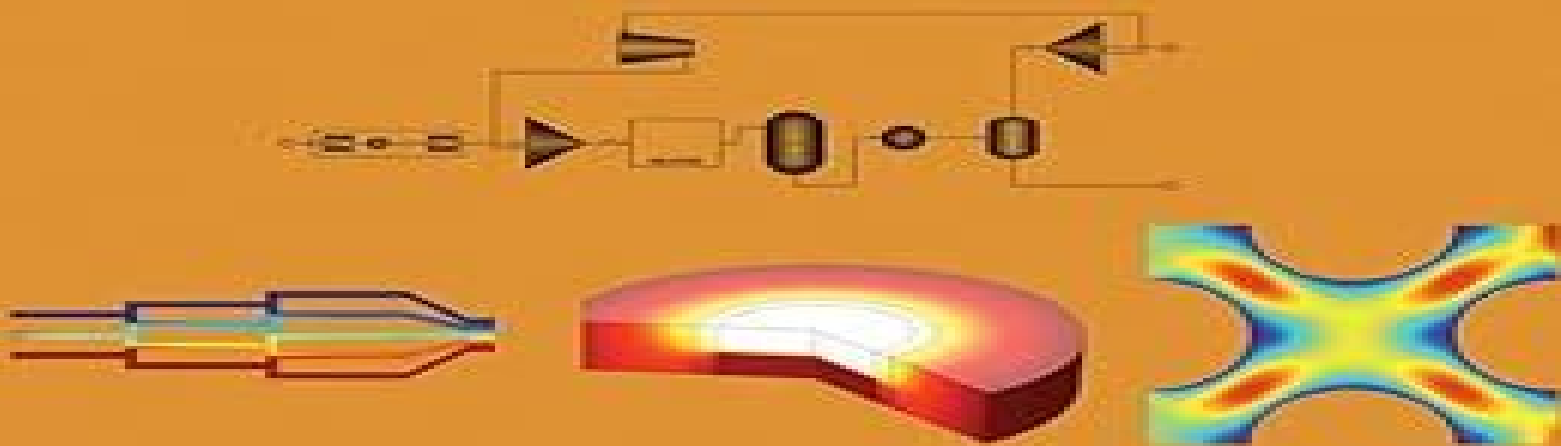


*Second Edition*

# Introduction to Chemical Engineering Computing

*Bruce A. Finlayson*



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**MATLAB Applications in Chemical Engineering** Chyi-Tsong Chen, 2022-05-20 This book addresses the applications of MATLAB and Simulink in the solution of chemical engineering problems By classifying the problems into seven different categories the author organizes this book as follows Chapter One Solution of a System of Linear Equations Chapter Two Solution of Nonlinear Equations Chapter Three Interpolation Differentiation and Integration Chapter Four Numerical Solution of Ordinary Differential Equations Chapter Five Numerical solution of Partial Differential Equations Chapter Six Process Optimization Chapter Seven Parameter Estimation Each chapter is arranged in four major parts In the first part the basic problem patterns that can be solved with MATLAB are presented The second part describes how to apply MATLAB commands to solve the formulated problems in the field of chemical engineering In the third and the fourth parts exercises and summary of MATLAB instructions are provided respectively The description of the chemical engineering example follows the sequence of problem formulation model

analysis MATLAB program design execution results and discussion In this way learners are first aware of the basic problem patterns and the underlying chemical engineering principles followed by further familiarizing themselves with the relevant MATLAB instructions and programming skills Readers are encouraged to do exercises to practice their problem solving skills and deepen the fundamental knowledge of chemical engineering and relevant application problems The table of contents is listed below Chapter 1 Solution of a System of Linear Equations 1 1 1 Properties of linear equation systems and the relevant MATLAB commands 1 1 2 Chemical engineering examples 10 1 3 Exercises 43 1 4 Summary of the MATLAB commands related to this chapter 48 Chapter 2 Solution of Nonlinear Equations 51 2 1 Relevant MATLAB commands and the Simulink solution interface 51 2 2 Chemical engineering examples 70 2 3 Exercises 103 2 4 Summary of MATLAB commands related to this chapter 122 Chapter 3 Interpolation Differentiation and Integration 125 3 1 Interpolation commands in MATLAB 125 3 2 Numerical differentiation 131 3 3 Numerical integration 153 3 4 Chemical engineering examples 157 3 5 Exercises 183 3 6 Summary of the MATLAB commands related to this chapter 195 Chapter 4 Numerical Solution of Ordinary Differential Equations 197 4 1 Initial value problems for ordinary differential equations 197 4 2 Higher order ordinary differential equations 222 4 3 Stiff differential equations 227 4 4 Differential algebraic equation system 232 4 5 Boundary valued ordinary differential equations 236 4 6 Chemical engineering examples 254 4 7 Exercises 285 4 8 Summary of the MATLAB commands related to this chapter 308 Chapter 5 Numerical Solution of Partial Differential Equations 311 5 1 Classifications of PDEs 311 5 2 The MATLAB PDE toolbox 316 5 3 Chemical engineering examples 341 5 4 Exercises 388 5 5 Summary of the MATLAB commands related to this chapter 397 Chapter 6 Process Optimization 399 6 1 The optimization problem and the relevant MATLAB commands 399 6 2 Chemical engineering examples 448 6 3 Exercises 481 6 4 Summary of the MATLAB commands related to this chapter 501 Chapter 7 Parameter Estimation 503 7 1 Parameter estimation using the least squares method 503 7 2 Chemical engineering examples 517 7 3 Exercises 549 7 4 Summary of the MATLAB commands related to this chapter 560 References 563 Index 569

### **Chemical Engineering Computation with MATLAB®** Yeong

Koo Yeo, 2017-08-01 Most problems encountered in chemical engineering are sophisticated and interdisciplinary Thus it is important for today's engineering students researchers and professionals to be proficient in the use of software tools for problem solving MATLAB is one such tool that is distinguished by the ability to perform calculations in vector matrix form a large library of built in functions strong structural language and a rich set of graphical visualization tools Furthermore MATLAB integrates computations visualization and programming in an intuitive user friendly environment Chemical Engineering Computation with MATLAB presents basic to advanced levels of problem solving techniques using MATLAB as the computation environment The book provides examples and problems extracted from core chemical engineering subject areas and presents a basic instruction in the use of MATLAB for problem solving It provides many examples and exercises and extensive problem solving instruction and solutions for various problems Solutions are developed using fundamental

principles to construct mathematical models and an equation oriented approach is used to generate numerical results A wealth of examples demonstrate the implementation of various problem solving approaches and methodologies for problem formulation problem solving analysis and presentation as well as visualization and documentation of results This book also provides aid with advanced problems that are often encountered in graduate research and industrial operations such as nonlinear regression parameter estimation in differential systems two point boundary value problems and partial differential equations and optimization

**Chemical Engineering Primer with Computer Applications** Hussein K.

Abdel-Aal, 2016-10-14 Taking a highly pragmatic approach to presenting the principles and applications of chemical engineering this companion text for students and working professionals offers an easily accessible guide to solving problems using computers The primer covers the core concepts of chemical engineering from conservation laws all the way up to chemical kinetics without heavy stress on theory and is designed to accompany traditional larger core texts The book presents the basic principles and techniques of chemical engineering processes and helps readers identify typical problems and how to solve them Focus is on the use of systematic algorithms that employ numerical methods to solve different chemical engineering problems by describing and transforming the information Problems are assigned for each chapter ranging from simple to difficult allowing readers to gradually build their skills and tackle a broad range of problems MATLAB and Excel are used to solve many examples and the more than 70 real examples throughout the book include computer or hand solutions or in many cases both The book also includes a variety of case studies to illustrate the concepts and a downloadable file containing fully worked solutions to the book's problems on the publisher's website Introduces the reader to chemical engineering computation without the distractions caused by the contents found in many texts Provides the principles underlying all of the major processes a chemical engineer may encounter as well as offers insight into their analysis which is essential for design calculations Shows how to solve chemical engineering problems using computers that require numerical methods using standard algorithms such as MATLAB and Excel Contains selective solved examples of many problems within the chemical process industry to demonstrate how to solve them using the techniques presented in the text Includes a variety of case studies to illustrate the concepts and a downloadable file containing fully worked solutions to problems on the publisher's website Offers non chemical engineers who are expected to work with chemical engineers on projects scale ups and process evaluations a solid understanding of basic concepts of chemical engineering analysis design and calculations

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AHUJA, PRADEEP, 2019-08-01 This book is an exhaustive presentation of the applications of numerical methods in chemical engineering Intended primarily as a textbook for B E B Tech and M Tech students of chemical engineering the book will also be useful for research and development process professionals in the fields of chemical biochemical mechanical and biomedical engineering The book now in its second edition comprises three parts Part I on General Chemical Engineering is

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understanding of the problems to prepare students for future challenging and innovative applications      *Mass Balances for Chemical Engineers* Gumersindo Feijoo, Juan Manuel Lema, Maria Teresa Moreira, 2020-07-20 The fundamentals of mass balances relevant for chemical engineers summarized in an easy comprehensible manner Plenty of example calculations schemes and flow diagrams facilitate the understanding Case studies from relevant topics such as sustainable chemistry illustrate the theory behind current applications      *Mathematical Modelling and Simulation in Chemical Engineering* M. Chidambaram, 2018-03-09 An easy to understand guide covering key principles of mathematical modelling and simulation in chemical engineering      **The Chemical Engineer** , 2009      **Fundamental Concepts and Computations in Chemical Engineering** Vivek Utgikar, 2016-10-25 The Breakthrough Introduction to Chemical Engineering for Today's Students Fundamental Concepts and Computations in Chemical Engineering is well designed for today's chemical engineering students offering lucid and logically arranged text that brings together the fundamental knowledge students need to gain confidence and to jumpstart future success Dr Vivek Utgikar illuminates the day to day roles of chemical engineers in their companies and in the global economy He clearly explains what students need to learn and why they need to learn it and presents practical computational exercises that prepare beginning students for more advanced study Utgikar combines straightforward discussions of essential topics with challenging topics to intrigue more well prepared students Drawing on extensive experience teaching beginners he introduces each new topic in simple relatable language and supports them with meaningful example calculations in Microsoft Excel and Mathcad Throughout Utgikar presents practical methods for effective problem solving and explains how to set up and use computation tools to get accurate answers Designed specifically for students entering chemical engineering programs this text also serves as a handy quick reference to the basics for more advanced students and an up to date source of valuable information for educators and professionals Coverage includes Where chemical engineering fits in the engineering field and overall economy Modern chemical engineering and allied industries and their largest firms How typical chemical engineering job functions build on what undergraduates learn The importance of computations and the use of modern computational tools How to classify problems based on their mathematical nature Fundamental fluid flow phenomena and computational problems in practical systems Basic principles and computations of material and energy balance Fundamental principles and calculations of thermodynamics and kinetics in chemical engineering How chemical engineering systems and problems integrate and interrelate in the real world Review of commercial process simulation software for complex large scale computation      *Introduction to Software for Chemical Engineers, Second Edition* Mariano Martín Martín, 2019-06-06 The field of Chemical Engineering and its link to computer science is in constant evolution and new engineers have a variety of tools at their disposal to tackle their everyday problems Introduction to Software for Chemical Engineers Second Edition provides a quick guide to the use of various computer packages for chemical engineering applications It covers a range of software applications from Excel and general

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