Second Edition

Introduction to Chemical Engineering Computing

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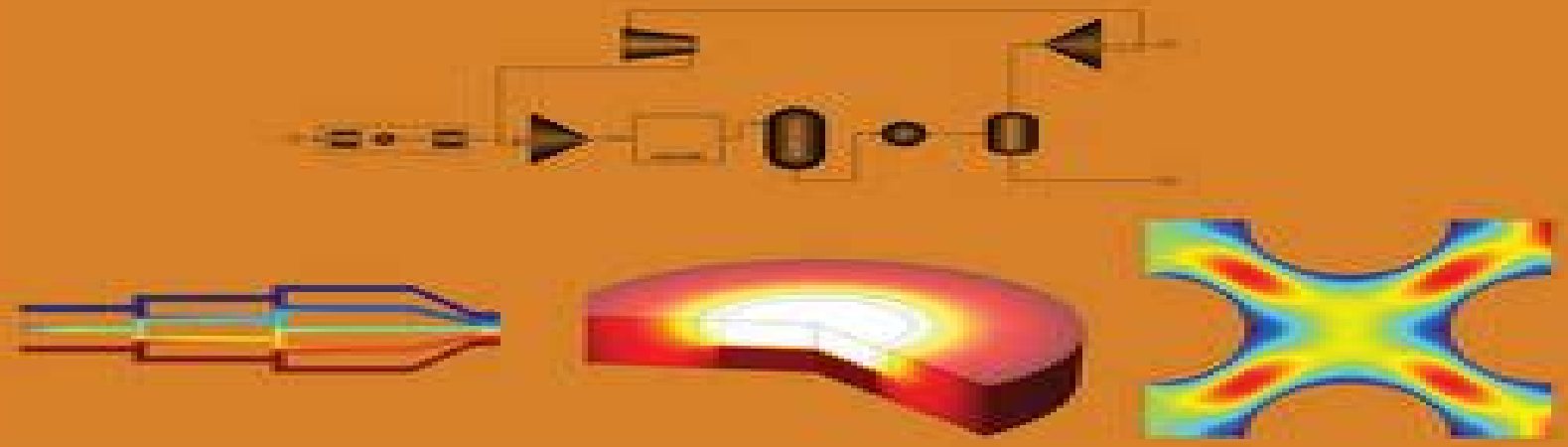
Bruce A. Finlayson



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Introduction to Chemical Engineering Computing Bruce A. Finlayson,2006-02-10 An innovative introduction to chemical engineering computing As chemical engineering technology advances so does the complexity of the problems that arise The problemsthat chemical engineers and chemical engineering students face today can no longer be answered with programs written on a case by case basis Introduction to Chemical Engineering Computing teaches professionalsand students the kinds of problems they will have to solve the types of computer programs needed to solve these problems and how to ensure that the problems have been solved correctly Each chapter in Introduction to Chemical Engineering Computing contains a description of the physicalproblem in general terms and in a mathematical context thorough step by step instructions numerous examples and comprehensive explanations for each problem and program This indispensable text features Excel MATLAB r Aspen PlusTM and FEMLAB programs and acquaints readers with the advantages of each Perfect for students and professionals Introduction to Chemical Engineering Computing gives readers the professional tools they need to solve real world problems involving Equations of state Vapor liquid and chemical reaction equilibria Mass balances with recycle streams Mass transfer equipment Process simulation Chemical reactors Transfer processes in 1D Fluid flow in 2D and 3D

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new and improving computer software Its user friendly approach to simulation and optimization as well as its example based presentation of the software makes it a perfect teaching tool for both undergraduate and master levels 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 MAT LAB 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

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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 **The Chemical Engineer** ,2009 **Introduction to Chemical Engineering Analysis Using Mathematica** Henry C. Foley,2021-06-16 Introduction to Chemical Engineering Analysis Using Mathematica Second Edition reviews the processes and designs used to manufacture use and dispose of chemical products using Mathematica one of the most powerful mathematical software tools available for symbolic numerical and graphical computing Analysis and computation are explained simultaneously The book covers the core concepts of chemical engineering ranging from the conservation of mass and energy to chemical kinetics The text also shows how to use the latest version of Mathematica from the basics of writing a few lines of code through developing entire analysis programs This second edition has been fully revised and updated and includes analyses of the conservation of energy whereas the first edition focused on the conservation of mass and ordinary differential equations Offers a fully revised and updated new edition extended with conservation of energy Covers a large

number of topics in chemical engineering analysis particularly for applications to reaction systems Includes many detailed examples Contains updated and new worked problems at the end of the book Written by a prominent scientist in the field

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