Second Edition

Introduction to Chemical Engineering Computing

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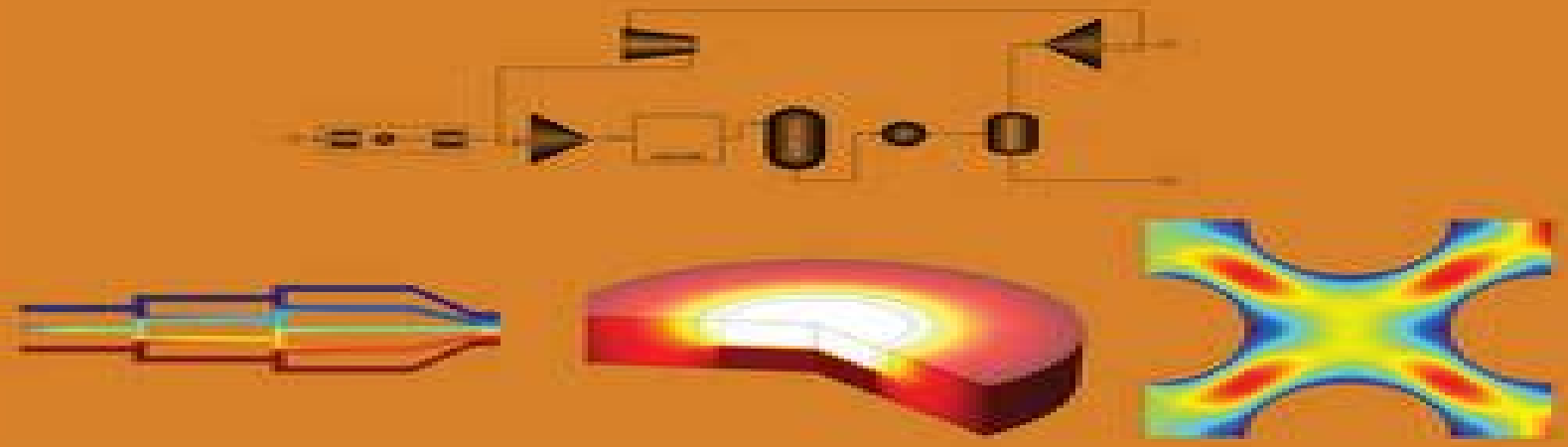
Bruce A. Finlayson



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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 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

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quick guide to the use of various computer packages for chemical engineering applications It covers a range of software applications including Excel and general mathematical packages such as MATLAB MathCAD R and Python Coverage also extends to process simulators such as CHEMCAD HYSYS and Aspen equation based modeling languages such as gPROMS optimization software such as GAMS AIMS and Julia and specialized software like CFD or DEM codes The different packages are introduced and applied to solve typical problems in fluid mechanics heat and mass transfer mass and energy balances unit operations reactor engineering and process and equipment design and control This new edition is updated throughout to reflect software updates and new packages It emphasizes the addition of SimaPro due to the importance of life cycle assessment as well as general statistics software SPSS and Minitab that readers can use to analyze lab data The book also includes new chapters on flowsheeting drawing process control and LOOP Pro as well as updates to include Pyomo as an optimization platform reflecting current trends The text offers a global idea of the capabilities of the software used in the chemical engineering field and provides examples for solving real world problems Written by leading experts this handbook is a must have reference for chemical engineers looking to grow in their careers through the use of 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 graduate level readers **Paperbound Books in Print** ,1992 **The British National Bibliography** Arthur James Wells,2006 **CJChE** ,2004-08 *Mechanical & Chemical Engineering Transactions* ,1965 New Technical Books New York Public Library,1925

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