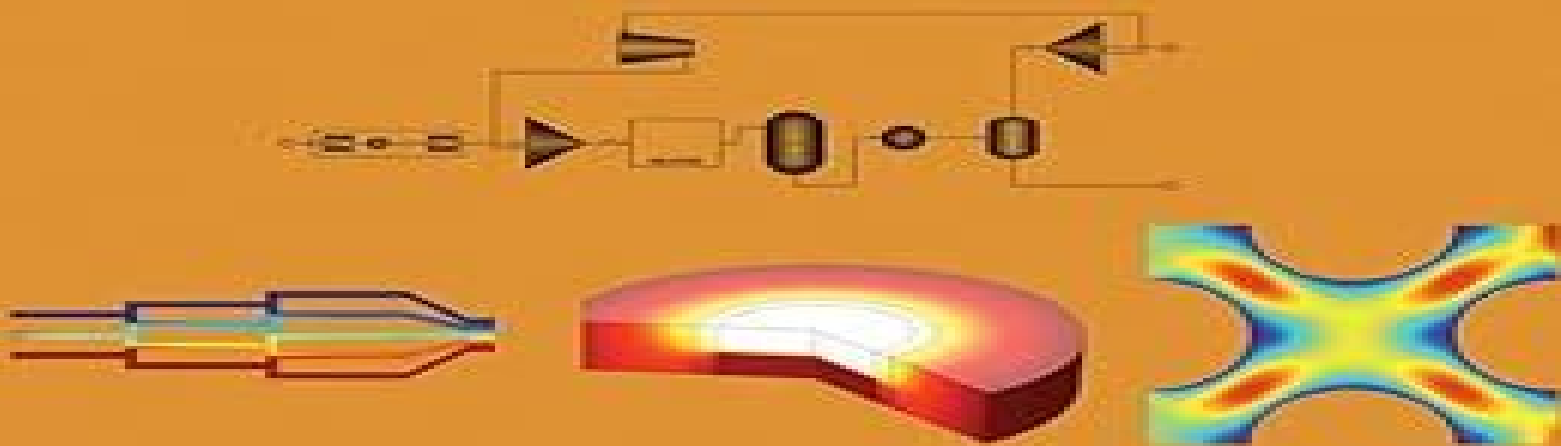


Second Edition

Introduction to Chemical Engineering Computing

Bruce A. Finlayson



Introduction To Chemical Engineering Computing 2nd Edition

Marcel Maeder, Yorck-Michael Neuhold



Introduction To Chemical Engineering Computing 2nd Edition:

Introduction to Chemical Engineering Computing Bruce A. Finlayson, 2014-03-05 Step by step instructions enable chemical engineers to master key software programs and solve complex problems Today both students and professionals in chemical engineering must solve increasingly complex problems dealing with refineries fuel cells microreactors and pharmaceutical plants to name a few With this book as their guide readers learn to solve these problems using their computers and Excel MATLAB Aspen Plus and COMSOL Multiphysics Moreover they learn how to check their solutions and validate their results to make sure they have solved the problems correctly Now in its Second Edition Introduction to Chemical Engineering Computing is based on the author's firsthand teaching experience As a result the emphasis is on problem solving Simple introductions help readers become conversant with each program and then tackle a broad range of problems in chemical engineering including Equations of state Chemical reaction equilibria Mass balances with recycle streams Thermodynamics and simulation of mass transfer equipment Process simulation Fluid flow in two and three dimensions All the chapters contain clear instructions figures and examples to guide readers through all the programs and types of chemical engineering problems Problems at the end of each chapter ranging from simple to difficult allow readers to gradually build their skills whether they solve the problems themselves or in teams In addition the book's accompanying website lists the core principles learned from each problem both from a chemical engineering and a computational perspective Covering a broad range of disciplines and problems within chemical engineering Introduction to Chemical Engineering Computing is recommended for both undergraduate and graduate students as well as practicing engineers who want to know how to choose the right computer software program and tackle almost any chemical engineering problem

Introduction to Chemical Engineering Computing Mr. Rohit Manglik, 2023-06-23 Introduces computing tools for chemical engineering applications problems Covers simulation software data analysis process modeling for design optimization in chemical industries plants manufacturing

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

Introduction to Process Control, Second Edition Jose A. Romagnoli, Ahmet Palazoglu, 2012-02-14

Introduction to Process Control Second Edition provides a bridge between the traditional view of process control and the current expanded role by blending conventional topics with a broader perspective of more integrated process operation control and information systems Updating and expanding the content of its predecessor this second edition addresses issues in today's teaching of process control Teaching Learning Principles Presents a concept first followed by an example allowing

students to grasp theoretical concepts in a practical manner Uses the same problem in each chapter culminating in a complete control design strategy Includes 50 percent more exercises Content Defines the traditional and expanded roles of process control in modern manufacturing Introduces the link between process optimization and process control optimizing control including the effect of disturbances on the optimal plant operation the concepts of steady state and dynamic backoff as ways to quantify the economic benefits of control and how to determine an optimal transition policy during a planned production change Incorporates an introduction to the modern architectures of industrial computer control systems with real case studies and applications to pilot scale operations Discusses the expanded role of process control in modern manufacturing including model centric technologies and integrated control systems Integrates data processing reconciliation and intelligent monitoring in the overall control system architecture Web Resource The book s website offers a user friendly software environment for interactively studying the examples in the text The site contains the MATLAB toolboxes for process control education as well as the main simulation examples from the book Access the site through the authors websites at www.pseonline.net and www.chms.ucdavis.edu/research/web_pse_ahmet Drawing on the authors combined 50 years of teaching experiences this classroom tested text is designed for chemical engineering students but is also suitable for industrial practitioners who need to understand key concepts of process control and how to implement them The authors help readers see how traditional process control has evolved into an integrated operational environment used to run modern manufacturing facilities

INTRODUCTION TO NUMERICAL METHODS IN CHEMICAL ENGINEERING, SECOND EDITION 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 same as given in the first edition of the book It explains solving linear and non linear algebraic equations chemical engineering thermodynamics problems initial value problems boundary value problems and topics related to chemical reaction dispersion and diffusion as well as steady and transient heat conduction Whereas Part II and Part III comprising two chapters and six chapters respectively are newly introduced in the present edition Besides three appendices covering computer programs have been included For practice the book provides students with numerous worked out examples and chapter end exercises including their answers NEW TO THE SECOND EDITION Part II on Fixed Bed Catalytic Reactor consists of solving multiple gas phase reactions in a PFR diffusion and multiple reactions in a catalytic pellet and fixed bed catalytic reactor with multiple reactions Part III on Multicomponent Distillation consists of solving vapour liquid liquid isothermal flash using NRTL model adiabatic flash using Wilson model bubble point method theta method and Naphtali Sandholm method for distillation using modified Raoult s law with Wilson activity coefficient model *Modeling and*

Simulation of Chemical Process Systems Nayef Ghasem, 2018-11-08 In this textbook the author teaches readers how to model and simulate a unit process operation through developing mathematical model equations solving model equations manually and comparing results with those simulated through software It covers both lumped parameter systems and distributed parameter systems as well as using MATLAB and Simulink to solve the system model equations for both Simplified partial differential equations are solved using COMSOL an effective tool to solve PDE using the fine element method This book includes end of chapter problems and worked examples and summarizes reader goals at the beginning of each chapter

Practical Data Analysis in Chemistry Marcel Maeder, Yorck-Michael Neuhold, 2007-08-10 The majority of modern instruments are computerised and provide incredible amounts of data Methods that take advantage of the flood of data are now available importantly they do not emulate graph paper analyses on the computer Modern computational methods are able to give us insights into data but analysis or data fitting in chemistry requires the quantitative understanding of chemical processes The results of this analysis allows the modelling and prediction of processes under new conditions therefore saving on extensive experimentation Practical Data Analysis in Chemistry exemplifies every aspect of theory applicable to data analysis using a short program in a Matlab or Excel spreadsheet enabling the reader to study the programs play with them and observe what happens Suitable data are generated for each example in short routines this ensuring a clear understanding of the data structure Chapter 2 includes a brief introduction to matrix algebra and its implementation in Matlab and Excel while Chapter 3 covers the theory required for the modelling of chemical processes This is followed by an introduction to linear and non linear least squares fitting each demonstrated with typical applications Finally Chapter 5 comprises a collection of several methods for model free data analyses Includes a solid introduction to the simulation of equilibrium processes and the simulation of complex kinetic processes Provides examples of routines that are easily adapted to the processes investigated by the reader Model based analysis linear and non linear regression and model free analysis are covered

Ludwig's Applied Process Design for Chemical and Petrochemical Plants Incorporating Process Safety Incidents A. Kayode Coker, 2024-07-10 Ludwig s Applied Process Design for Chemical and Petrochemical Plants Incorporating Process Safety Incidents is ever evolving starting with the first edition some 60 years ago The volumes in this fifth edition provide improved techniques and fundamental design methodologies to guide the practicing engineer in designing process equipment and applying chemical processes to the properly detailed hardware As indicative of the new title process safety incidents are incorporated in many of the chapters reviewing the root causes and how these could be mitigated in future Like its predecessor this new edition continues to present updated information for achieving optimum operational and process conditions and to avoid problems caused by inadequate sizing and lack of internally detailed hardware The volumes provide both fundamental theories where applicable and direct application of these theories to applied equations essential in the design effort This approach in presenting design information is essential for troubleshooting process equipment and in

executing system performance analysis Volume 1B continues to cover mixing of liquids process safety and pressure 1 relieving devices metallurgy and corrosion and process optimization It builds upon Ernest E Ludwig s classic text to further enhance its use as a chemical engineering process design manual of methods and proven fundamentals This new edition includes new content on three phase separation mixing of liquids ejectors and mechanical vacuum systems process safety and pressure relieving devices metallurgy and corrosion and optimization of chemical process blending Some chapters review pressure relieving devices and provide case studies for process safety incidents which are well illustrated from US Chemical Safety Hazard Investigation Board www.csb.gov Finally this book contains a glossary of Petroleum and Petrochemical Terminologies and Physical and Chemical Characteristics of Major Hydrocarbons Provides improved design manual for methods and proven fundamentals of process design with related data and charts Covers complete range of basic day to day petrochemical operation topics Extensively revised with new material added on three phase separation metallurgy and corrosion Process safety management HAZOP and hazard analyses and optimization of chemical process blending Presents many examples using Honeywell UniSim Design software developed and executable computer programs and Excel spreadsheet programs Includes case studies of process safety incidents guidance for troubleshooting and checklists Includes Software of Conversion Table and 30 process data sheets in excel format

Ludwig's Applied Process Design for Chemical and Petrochemical Plants A. Kayode Coker, 2011-08-30 This complete revision of Applied Process Design for Chemical and Petrochemical Plants Volume 1 builds upon Ernest E Ludwig s classic text to further enhance its use as a chemical engineering process design manual of methods and proven fundamentals This new edition includes important supplemental mechanical and related data nomographs and charts Also included within are improved techniques and fundamental methodologies to guide the engineer in designing process equipment and applying chemical processes to properly detailed equipment All three volumes of Applied Process Design for Chemical and Petrochemical Plants serve the practicing engineer by providing organized design procedures details on the equipment suitable for application selection and charts in readily usable form Process engineers designers and operators will find more chemical petrochemical plant design data in Volume 2 Third Edition which covers distillation and packed towers as well as material on azeotropes and ideal non ideal systems Volume 3 Third Edition which covers heat transfer refrigeration systems compression surge drums and mechanical drivers A Kayode Coker is Chairman of Chemical Process Engineering Technology department at Jubail Industrial College in Saudi Arabia He s both a chartered scientist and a chartered chemical engineer for more than 15 years and an author of Fortran Programs for Chemical Process Design Analysis and Simulation Gulf Publishing Co and Modeling of Chemical Kinetics and Reactor Design Butterworth Heinemann Provides improved design manuals for methods and proven fundamentals of process design with related data and charts Covers a complete range of basic day to day petrochemical operation topics with new material on significant industry changes since 1995

Mathematical Methods in Chemical and Biological

Engineering Binay Kanti Dutta, 2016-11-03 Mathematical Methods in Chemical and Biological Engineering describes basic to moderately advanced mathematical techniques useful for shaping the model based analysis of chemical and biological engineering systems. Covering an ideal balance of basic mathematical principles and applications to physico chemical problems, this book presents examples drawn from recent scientific and technical literature on chemical engineering, biological and biomedical engineering, food processing and a variety of diffusional problems to demonstrate the real world value of the mathematical methods. Emphasis is placed on the background and physical 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 Written in a clear logical and concise manner, this comprehensive resource provides discussion on essential mathematical tools required for upgraded system performance. Understanding of basic principles and governing laws is essential to reduce complexity of the system and this guide offers detailed discussion on analytical and numerical techniques to solve mathematical model equations. Important concepts including nonlinear algebraic equations, initial value ordinary differential equations (ODEs) and boundary value ODEs are discussed in detail. The concepts of optimization methods and sensitivity analysis, which are important from subject point of view, are explained with suitable examples. Numerous problems and MATLAB/Scilab exercises are interspersed throughout the text. Several case studies involving full details of simulation are offered for better understanding. The accompanying website will host additional MATLAB/Scilab problems, model question papers, simulation exercises, tutorials and projects. This book will be useful for students of chemical engineering, mechanical engineering, instrumentation engineering and mathematics. **Computational Fluid Dynamics and COMSOL**

Multiphysics Ashish S. Chaurasia, 2021-12-29 This textbook covers computational fluid dynamics simulation using COMSOL Multiphysics Modeling Software in chemical engineering applications. In the volume, the COMSOL Multiphysics package is introduced and applied to solve typical problems in chemical reactors, transport processes, fluid flow and heat and mass transfer. Inspired by the difficulties of introducing the use of COMSOL Multiphysics software during classroom time, the book incorporates the author's experience of working with undergraduate, graduate and postgraduate students to make the book user friendly and that at the same time addresses typical examples within the subjects covered in the chemical engineering curriculum. Real world problems require the use of simulation and optimization tools and this volume shows how COMSOL Multiphysics software can be used for that purpose. Key features: Includes over 500 step by step screenshots. Shows the graphical user interface of COMSOL which does not require any programming effort. Provides chapter end problems for

extensive practice along with solutions Includes actual examples of chemical reactors transport processes fluid flow and heat and mass transfer This book is intended for students who want or need more help to solve chemical engineering assignments using computer software It can also be used for computational courses in chemical engineering It will also be a valuable resource for professors research scientists and practicing engineers *Micro Instrumentation* Melvin V. Koch, Kurt M. VandenBussche, Ray W. Chrisman, 2007-06-27 This first comprehensive treatment of the intertwined roles of micro instrumentation high throughput experimentation and process intensification as valuable tools for process analytical technology covers both industrial as well as academic aspects First class editors and authors from top companies and universities provide interdisciplinary coverage ranging from chemistry and analytics to process design and engineering supported throughout by case studies and ample analytical data **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 mathematical packages such as MATLAB and MathCAD to process simulators CHEMCAD and ASPEN equation based modeling languages gProms optimization software such as GAMS and AIMS 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 process and equipment design and control This new edition offers a wider view of packages including open source software such as R Python and Julia It also includes complete examples in ASPEN Plus adds ANSYS Fluent to CFD codes Lingo to the optimization packages and discusses Engineering Equation Solver It 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 book 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 master levels **Chemical Engineering Progress**,2006

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