

# Computer Methods In Chemical Engineering Nayef Ghasem

Molecular Modeling and Theory in Chemical Engineering  
Introduction to Chemical Engineering Computing  
26th European Symposium on Computer Aided Process Engineering  
Applied Mathematical Methods for Chemical Engineers  
Exam Prep for: Computer Methods in Chemical Engineering  
Chemical Engineering Computation with MATLAB®  
Mathematical Methods in Chemical Engineering  
Exam Prep for: Computer Methods in Chemical Engineering  
Software Architectures and Tools for Computer Aided Process Engineering  
On-Line Computer Methods relevant to chemical engineering  
Chemical Engineering Primer with Computer Applications  
Computational Methods in Reactor Shielding  
Computer Methods in Chemical Engineering  
Integrated Design and Simulation of Chemical Processes  
Introduction to Software for Chemical Engineers, Second Edition  
Computational Techniques for Chemical Engineers  
Numerical Methods for Chemical Engineering  
The Integration of Process Design and Control  
Numerical Methods for Chemical Engineers Using Excel, VBA, and MATLAB  
Modeling and Simulation of Chemical Process Systems  
24th European Symposium on Computer Aided Process Engineering  
MATHEMATICAL METHODS IN CHEMICAL ENGINEERING  
20th European Symposium of Computer Aided Process Engineering  
Advanced Data Analysis and Modelling in Chemical Engineering  
Principles of Chemical Engineering Processes  
Research Methods and Applications in Chemical and Biological Engineering  
Online Computer Methods Relevant to Chemical Engineering  
Chemical Process Design  
Computational Methods in Chemical Engineering  
Chemical Nanoscience and Nanotechnology  
Efficient Computer Methods for the Practising Chemical Engineer  
Practical Numerical Methods for Chemical Engineers  
Computer Methods in Chemical Engineering  
Numerical Methods and Modeling for Chemical Engineers  
Computer Methods in Chemical Engineering  
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Computational Methods for Process Simulation  
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12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering

## Molecular Modeling and Theory in Chemical Engineering

ESCAPE-20 is the most recent in a series of conferences that serves as a forum for engineers, scientists, researchers, managers and students from academia and industry to present and discuss progress being made in the area of "Computer Aided Process Engineering" (CAPE). CAPE covers computer-aided methods, algorithms and techniques related to process and product engineering. The ESCAPE-20 scientific program reflects the strategic objectives of the CAPE Working Party: to check the status of historically consolidated topics by means of their industrial application and to evaluate their emerging issues. \* Includes a CD that contains all research papers and contributions \* Features a truly international scope, with guest speakers and keynote talks from leaders in science and industry \* Presents papers covering the latest research, key topical areas, and developments in computer-aided process engineering (CAPE)

## **Introduction to Chemical Engineering Computing**

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.

## **26th European Symposium on Computer Aided Process Engineering**

### **Applied Mathematical Methods for Chemical Engineers**

Authors Owen Hanna and Orville Sandall include broad use of convergence acceleration techniques such as Pade approximation for series; Shanks transformation for series; linear and nonlinear systems of algebraic equations; systematic use of global Richardson extrapolation for integrals and ODE systems to monitor the overall error; and discussion of methods for the solution of stiff ODE.

### **Exam Prep for: Computer Methods in Chemical Engineering**

26th European Symposium on Computer Aided Process Engineering contains the papers presented at the 26th European Society of Computer-Aided Process

Engineering (ESCAPE) Event held at Portorož Slovenia, from June 12th to June 15th, 2016. Themes discussed at the conference include Process-product Synthesis, Design and Integration, Modelling, Numerical analysis, Simulation and Optimization, Process Operations and Control and Education in CAPE/PSE. Presents findings and discussions from the 26th European Society of Computer-Aided Process Engineering (ESCAPE) Event

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

Computational Methods in Reactor Shielding deals with the mathematical processes involved in how to effectively control the dangerous effect of nuclear radiation. Reactor shielding is considered an important aspect in the operation of reactor systems to ensure the safety of personnel and others that can be directly or indirectly affected. Composed of seven chapters, the book discusses ionizing radiation and how it aids in the control and containment of radioactive substances that are considered harmful to all living things. The text also outlines the necessary radiation quantities and units that are needed for a systemic control of shielding and presents an examination of the main sources of nuclear radiation. A discussion of the gamma photon cross sections and an introduction to BMIX, a computer program used in illustrating a technique in identifying the gamma ray build-up factor for a reactor shield, are added. The selection also discusses various mathematical representations and areas of shielding theory that are being used in radiation shielding. The book is of great value to those involved in the development and implementation of systems to minimize and control the dangerous and lethal effect of radiation.

## **Mathematical Methods in Chemical Engineering**

Step-by-step instructions enable chemical engineers to masterkey 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.

## **Exam Prep for: Computer Methods in Chemical Engineering**

This comprehensive, well organized and easy to read book presents concepts in a unified framework to establish a similarity in the methods of solutions and analysis of such diverse systems as algebraic equations, ordinary differential equations and partial differential equations. The distinguishing feature of the book is the clear focus on analytical methods of solving equations. The text explains how the methods meant to elucidate linear problems can be extended to analyse nonlinear problems. The book also discusses in detail modern concepts like bifurcation theory and chaos. To attract engineering students to applied mathematics, the author explains the concepts in a clear, concise and straightforward manner, with the help of examples and analysis. The significance of analytical methods and concepts for the engineer/scientist interested in numerical applications is clearly brought out. Intended as a textbook for the postgraduate students in engineering, the book could also be of great help to the research students.

## **Software Architectures and Tools for Computer Aided Process Engineering**

This text introduces the quantitative treatment of differential equations arising from modeling physical phenomena in chemical engineering. Coverage includes recent topics such as ODE-IVPs, emphasizing numerical methods and modeling of 1984-era commercial mathematical software.

## **On-Line Computer Methods relevant to chemical engineering**

## **Chemical Engineering Primer with Computer Applications**

## **Computational Methods in Reactor Shielding**

Applications of numerical mathematics and scientific computing to chemical engineering.

## **Computer Methods in Chemical Engineering**

While various software packages have become quite useful for performing unit operations and other kinds of processes in chemical engineering, the fundamental theory and methods of calculation must also be understood in order to effectively test the validity of these packages and verify the results. Computer Methods in Chemical Engineering presents the most commonly used simulation software, along with the theory involved. It covers chemical engineering thermodynamics, fluid mechanics, material and energy balances, mass transfer operations, reactor design, and computer applications in chemical engineering. Through this book,

students learn: What chemical engineers do The functions and theoretical background of basic chemical engineering unit operations How to simulate chemical processes using software packages How to size chemical process units manually and with software How to fit experimental data How to solve linear and nonlinear algebraic equations as well as ordinary differential equations Along with exercises and references, each chapter contains a theoretical description of process units followed by numerous examples that are solved step by step via hand calculations and computer simulation using Hysys/Unisim, PRO/II, Aspen Plus, and SuperPro Designer. Adhering to the Accreditation Board for Engineering and Technology (ABET) criteria, the book gives students the tools needed to solve real problems involving thermodynamics and fluid-phase equilibria, fluid flow, material and energy balances, heat exchangers, reactor design, distillation, absorption, and liquid-liquid extraction.

## **Integrated Design and Simulation of Chemical Processes**

This research-oriented book presents up-to-date experimental methods currently used in research for many branches of chemical and biological engineering. The book surveys essential ideas and research methodologies, concentrating on experiments used in applications rather than on the fine points of rigorous mathematics. Examples of important applications are reviewed in sufficient detail to provide the reader with a critical understanding of context and research methodology. The volume presents a broad spectrum of chapters in the various branches of chemical and biological engineering that demonstrate key developments in these rapidly changing fields. Chapters explore the design, development, operation, monitoring, control, and optimization of chemical, physical and biological processes. Case studies are included in some chapters, building a real-world connection.

## **Introduction to Software for Chemical Engineers, Second Edition**

While various software packages have become quite useful for performing unit operations and other kinds of processes in chemical engineering, the fundamental theory and methods of calculation must also be understood in order to effectively test the validity of these packages and verify the results. Computer Methods in Chemical Engineering presents the most commonly used simulation software, along with the theory involved. It covers chemical engineering thermodynamics, fluid mechanics, material and energy balances, mass transfer operations, reactor design, and computer applications in chemical engineering. Through this book, students learn: What chemical engineers do The functions and theoretical background of basic chemical engineering unit operations How to simulate chemical processes using software packages How to size chemical process units manually and with software How to fit experimental data How to solve linear and nonlinear algebraic equations as well as ordinary differential equations Along with exercises and references, each chapter contains a theoretical description of process units followed by numerous examples that are solved step by step via hand calculations and computer simulation using Hysys/Unisim, PRO/II, Aspen Plus, and SuperPro Designer. Adhering to the Accreditation Board for Engineering and

Technology (ABET) criteria, the book gives students the tools needed to solve real problems involving thermodynamics and fluid-phase equilibria, fluid flow, material and energy balances, heat exchangers, reactor design, distillation, absorption, and liquid-liquid extraction.

## **Computational Techniques for Chemical Engineers**

In recent years chemical engineers have become increasingly involved in the design and synthesis of new materials and products as well as the development of biological processes and biomaterials. Such applications often demand that product properties be controlled with precision. Molecular modeling, simulating chemical and molecular structures or processes by computer, aids scientists in this endeavor. Volume 28 of *Advances in Chemical Engineering* presents discussions of theoretical and computational methods as well as their applications to specific technologies.

## **Numerical Methods for Chemical Engineering**

This book presents Maple solutions to a wide range of problems relevant to chemical engineers and others. Many of these solutions use Maple's symbolic capability to help bridge the gap between analytical and numerical solutions. The readers are strongly encouraged to refer to the references included in the book for a better understanding of the physics involved, and for the mathematical analysis. This book was written for a senior undergraduate or a first year graduate student course in chemical engineering. Most of the examples in this book were done in Maple 10. However, the codes should run in the most recent version of Maple. We strongly encourage the readers to use the classic worksheet (\*.mws) option in Maple as we believe it is more user-friendly and robust. In chapter one you will find an introduction to Maple which includes simple basics as a convenience for the reader such as plotting, solving linear and nonlinear equations, Laplace transformations, matrix operations, 'do loop,' and 'while loop.' Chapter two presents linear ordinary differential equations in section 1 to include homogeneous and nonhomogeneous ODEs, solving systems of ODEs using the matrix exponential and Laplace transform method. In section two of chapter two, nonlinear ordinary differential equations are presented and include simultaneous series reactions, solving nonlinear ODEs with Maple's 'dsolve' command, stop conditions, differential algebraic equations, and steady state solutions. Chapter three addresses boundary value problems.

## **The Integration of Process Design and Control**

Chemistry and chemical engineering have changed significantly in the last decade. They have broadened their scope into biology, nanotechnology, materials science, computation, and advanced methods of process systems engineering and control so much that the programs in most chemistry and chemical engineering departments now barely resemble the classical notion of chemistry. Beyond the Molecular Frontier brings together research, discovery, and invention across the entire spectrum of the chemical sciences from fundamental, molecular-level chemistry to large-scale chemical processing technology. This reflects the way the

field has evolved, the synergy at universities between research and education in chemistry and chemical engineering, and the way chemists and chemical engineers work together in industry. The astonishing developments in science and engineering during the 20th century have made it possible to dream of new goals that might previously have been considered unthinkable. This book identifies the key opportunities and challenges for the chemical sciences, from basic research to societal needs and from terrorism defense to environmental protection, and it looks at the ways in which chemists and chemical engineers can work together to contribute to an improved future.

## **Numerical Methods for Chemical Engineers Using Excel, VBA, and MATLAB**

25th European Symposium on Computer-Aided Process Engineering contains the papers presented at the 12th Process Systems Engineering (PSE) and 25th European Society of Computer Aided Process Engineering (ESCAPE) Joint Event held in Copenhagen, Denmark, 31 May - 4 June 2015. The purpose of these series is to bring together the international community of researchers and engineers who are interested in computing-based methods in process engineering. This conference highlights the contributions of the PSE/CAPE community towards the sustainability of modern society. Contributors from academia and industry establish the core products of PSE/CAPE, define the new and changing scope of our results, and future challenges. Plenary and keynote lectures discuss real-world challenges (globalization, energy, environment, and health) and contribute to discussions on the widening scope of PSE/CAPE versus the consolidation of the core topics of PSE/CAPE. Highlights how the Process Systems Engineering/Computer-Aided Process Engineering community contributes to the sustainability of modern society Presents findings and discussions from both the 12th Process Systems Engineering (PSE) and 25th European Society of Computer-Aided Process Engineering (ESCAPE) Events Establishes the core products of Process Systems Engineering/Computer Aided Process Engineering Defines the future challenges of the Process Systems Engineering/Computer Aided Process Engineering community

## **Modeling and Simulation of Chemical Process Systems**

The 24th European Symposium on Computer Aided Process Engineering creates an international forum where scientific and industrial contributions of computer-aided techniques are presented with applications in process modeling and simulation, process synthesis and design, operation, and process optimization. The organizers have broadened the boundaries of Process Systems Engineering by inviting contributions at different scales of modeling and demonstrating vertical and horizontal integration. Contributions range from applications at the molecular level to the strategic level of the supply chain and sustainable development. They cover major classical themes, at the same time exploring a new range of applications that address the production of renewable forms of energy, environmental footprints and sustainable use of resources and water.

## **24th European Symposium on Computer Aided Process Engineering**

Principles of Chemical Engineering Processes: Material and Energy Balances introduces the basic principles and calculation techniques used in the field of chemical engineering, providing a solid understanding of the fundamentals of the application of material and energy balances. Packed with illustrative examples and case studies, this book: Discusses problems in material and energy balances related to chemical reactors Explains the concepts of dimensions, units, psychrometry, steam properties, and conservation of mass and energy Demonstrates how MATLAB® and Simulink® can be used to solve complicated problems of material and energy balances Shows how to solve steady-state and transient mass and energy balance problems involving multiple-unit processes and recycle, bypass, and purge streams Develops quantitative problem-solving skills, specifically the ability to think quantitatively (including numbers and units), the ability to translate words into diagrams and mathematical expressions, the ability to use common sense to interpret vague and ambiguous language in problem statements, and the ability to make judicious use of approximations and reasonable assumptions to simplify problems This Second Edition has been updated based upon feedback from professors and students. It features a new chapter related to single- and multiphase systems and contains additional solved examples and homework problems. Educational software, downloadable exercises, and a solutions manual are available with qualifying course adoption.

## **MATHEMATICAL METHODS IN CHEMICAL ENGINEERING**

While teaching the Numerical Methods for Engineers course over the last 15 years, the author found a need for a new textbook, one that was less elementary, provided applications and problems better suited for chemical engineers, and contained instruction in Visual Basic® for Applications (VBA). This led to six years of developing teaching notes that have been enhanced to create the current textbook, Numerical Methods for Chemical Engineers Using Excel®, VBA, and MATLAB®. Focusing on Excel gives the advantage of it being generally available, since it is present on every computer—PC and Mac—that has Microsoft Office installed. The VBA programming environment comes with Excel and greatly enhances the capabilities of Excel spreadsheets. While there is no perfect programming system, teaching this combination offers knowledge in a widely available program that is commonly used (Excel) as well as a popular academic software package (MATLAB). Chapters cover nonlinear equations, Visual Basic, linear algebra, ordinary differential equations, regression analysis, partial differential equations, and mathematical programming methods. Each chapter contains examples that show in detail how a particular numerical method or programming methodology can be implemented in Excel and/or VBA (or MATLAB in chapter 10). Most of the examples and problems presented in the text are related to chemical and biomolecular engineering and cover a broad range of application areas including thermodynamics, fluid flow, heat transfer, mass transfer, reaction kinetics, reactor design, process design, and process control. The chapters feature "Did You Know" boxes, used to remind readers of Excel features. They also contain end-of-chapter exercises, with solutions provided.

## **20th European Symposium of Computer Aided Process Engineering**

Process Modelling and simulation have proved to be extremely successful engineering tools for the design and optimisation of physical, chemical and biochemical processes. The use of simulation has expanded rapidly over the last two decades because of the availability of large high-speed computers and indeed has become even more widespread with the rise of the desk-top PC resources now available to nearly every engineer and student. In the chemical industry large, realistic non-linear problems are routinely solved with the aid of computer simulation. This has a number of benefits, including easy assessment of the economic desirability of a project, convenient investigation of the effects of changes to system variables, and finally the introduction of mathematical rigour into the design process and inherent assumptions that may not have been there before. Computational Methods for Process Simulation develops the methods needed for the simulation of real processes to be found in the process industries. It also stresses the engineering fundamentals used in developing process models. Steady state and dynamic systems are considered, for both spatially lumped and spatially distributed problems. It develops analytical and numerical computational techniques for algebraic, ordinary and partial differential equations, and makes use of computer software routines that are widely available. Dedicated software examples are available via the internet. Written for a compulsory course element in the US Includes examples using software used in academia and industry Software available via the Internet

## **Advanced Data Analysis and Modelling in Chemical Engineering**

### **Principles of Chemical Engineering Processes**

This latest 3rd edition expands the breadth of Practical Numerical Methods with over 100 VBA macros for extending Excel's power for engineering and scientific analysis. Engineers and scientists will find the enhanced coverage of computational tools applicable to a variety of problems in their own disciplines. \*\* The selection of software reflects Excel's status as the de facto computational tool used by practicing engineers. Engineers & scientists should become proficient at extending Excel's capabilities with VBA programming to boost their worksheets with time saving enhancements and powerful numerical techniques. \*\* Topics include an introduction to modeling, documentation, Excel & VBA, root-finding for linear & nonlinear systems of equations, multivariate optimization, experimental uncertainty propagation & analysis, least-squares regression & model validation, interpolation, integration, and ordinary & partial differential equations. \*\* A companion web site has links to digital files for downloading up to 200 illustrations & examples & the refined PNM3Suite workbook with VBA user-defined functions, macros, & user forms for advanced numerical techniques. Practice problems are also available from the web site (<https://www.d.umn.edu/~rdavis/PNM/PNMExcelVBA3/>). Example files & macros are ready to be modified by users for their own needs. \*\* Chapter 1 includes a brief introduction to chemical reaction engineering that provides some background needed for problems involving mass & energy balances with reactions. \*\* The next two chapters introduce frequently overlooked features of Excel and VBA for engineering programming to apply numerical methods in Excel, as well as document results.

The remaining chapters present powerful numerical techniques using Excel & VBA, including: \*\* General Methods: Sub & User-defined Function Procedures, Pseudo-random Number Generation, Sorting, Formula Graphing & Evaluation, Random Sampling, User forms \*\* Linear Equations: Gaussian Elimination with Maximum Column Pivoting, Error Correction, Crout Reduction, Thomas algorithm for tri-diagonal & Cholesky's method for symmetric matrices, Matrix functions, Jacobi & Gauss-Seidel Iteration, Wegstein & Steffenson's version of Aitkin's Delta Square methods, Power method for Eigenproblems \*\* Nonlinear Equations: Ordinary Fixed-Point Iteration, Bisection, Secant, Regula Falsi, Newton & Quasi-Newton, Continuation (homotopy), Goal Seek, Solver, Bairstow's method for polynomial roots \*\* Derivative Approximation: Finite Difference, Richardson's extrapolation, Jacobian, Sensitivity Analysis, Lagrange polynomials, splines \*\* Uncertainty Analysis: Jitter method for the Law of Propagation of Uncertainty, Monte Carlo with Latin-Hypercube sampling, Jack knife for regression parameter uncertainty \*\* Optimization: Graphical, Quadratic with acceleration, Powell, Golden Section, Luus-Jaakola, Solver (for linear and nonlinear programming), Parameter Scaling \*\* Least-squares Regression: multivariate linear models, Gauss-Newton, Levenberg-Marquardt, and Monte Carlo for nonlinear regression with parameter uncertainty, Rational Least Squares, Weighting \*\* Interpolation: Linear, Newton Divided Difference, Lagrange, Rational, Stineman, Cubic Spline, Constrained Splines, Bivariate 2-D, Data Smoothing \*\* Integration: Trapezoid, Improper, Midpoint, Romberg, Adaptive Gauss-Kronrod & Simpson, Splines, multiple integrals with Simpson, Kronrod, & Monte Carlo methods \*\* Initial-Value ODEs: Taylor Series, improved & modified Euler, implicit Trapezoidal for stiff problems, fixed & variable single step 4-5 order Runge-Kutta, Cash-Karp & Dormand-Prince, Adams-Bashforth-Moulton multi-step methods \*\* Boundary Value ODEs and PDEs: Shooting, Finite Difference, Collocation on Finite Elements, Quasilinearization, Method of Lines, semi-implicit Crank-Nicholson methods \*\* Tables for quick reference of Excel, VBA, and custom functions & macros for numerical m

## **Research Methods and Applications in Chemical and Biological Engineering**

Advanced Data Analysis and Modeling in Chemical Engineering provides the mathematical foundations of different areas of chemical engineering and describes typical applications. The book presents the key areas of chemical engineering, their mathematical foundations, and corresponding modeling techniques. Modern industrial production is based on solid scientific methods, many of which are part of chemical engineering. To produce new substances or materials, engineers must devise special reactors and procedures, while also observing stringent safety requirements and striving to optimize the efficiency jointly in economic and ecological terms. In chemical engineering, mathematical methods are considered to be driving forces of many innovations in material design and process development. Presents the main mathematical problems and models of chemical engineering and provides the reader with contemporary methods and tools to solve them Summarizes in a clear and straightforward way, the contemporary trends in the interaction between mathematics and chemical engineering vital to chemical engineers in their daily work Includes classical analytical methods, computational methods, and methods of symbolic computation Covers the latest cutting edge computational methods, like symbolic computational methods

## **Online Computer Methods Relevant to Chemical Engineering**

This practical how-to-do book deals with the design of sustainable chemical processes by means of systematic methods aided by computer simulation. Ample case studies illustrate generic creative issues, as well as the efficient use of simulation techniques, with each one standing for an important issue taken from practice. The didactic approach guides readers from basic knowledge to mastering complex flow-sheets, starting with chemistry and thermodynamics, via process synthesis, efficient use of energy and waste minimization, right up to plant-wide control and process dynamics. The simulation results are compared with flow-sheets and performance indices of actual industrial licensed processes, while the complete input data for all the case studies is also provided, allowing readers to reproduce the results with their own simulators. For everyone interested in the design of innovative chemical processes.

## **Chemical Process Design**

The idea of editing a book on modern software architectures and tools for CAPE (Computer Aided Process Engineering) came about when the editors of this volume realized that existing titles relating to CAPE did not include references to the design and development of CAPE software. Scientific software is needed to solve CAPE related problems by industry/academia for research and development, for education and training and much more. There are increasing demands for CAPE software to be versatile, flexible, efficient, and reliable. This means that the role of software architecture is also gaining increasing importance. Software architecture needs to reconcile the objectives of the software; the framework defined by the CAPE methods; the computational algorithms; and the user needs and tools (other software) that help to develop the CAPE software. The object of this book is to bring to the reader, the software side of the story with respect to computer aided process engineering.

## **Computational Methods in Chemical Engineering**

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.

## **Chemical Nanoscience and Nanotechnology**

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.

## **Efficient Computer Methods for the Practising Chemical Engineer**

This comprehensive work shows how to design and develop innovative, optimal and sustainable chemical processes by applying the principles of process systems engineering, leading to integrated sustainable processes with 'green' attributes. Generic systematic methods are employed, supported by intensive use of computer simulation as a powerful tool for mastering the complexity of physical models. New to the second edition are chapters on product design and batch processes with applications in specialty chemicals, process intensification methods for designing compact equipment with high energetic efficiency, plantwide control for managing the key factors affecting the plant dynamics and operation, health, safety and environment issues, as well as sustainability analysis for achieving high environmental performance. All chapters are completely rewritten or have been revised. This new edition is suitable as teaching material for Chemical Process and Product Design courses for graduate MSc students, being compatible with academic requirements world-wide. The inclusion of the newest design methods will be of great value to professional chemical engineers. Systematic approach to developing innovative and sustainable chemical processes Presents generic principles of process simulation for analysis, creation and assessment Emphasis on sustainable development for the future of process industries

## **Practical Numerical Methods for Chemical Engineers**

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.

## **Computer Methods in Chemical Engineering**

While various software packages have become quite useful for performing unit operations and other kinds of processes in chemical engineering, the fundamental theory and methods of calculation must also be understood in order to effectively test the validity of these packages and verify the results. Computer Methods in Chemical Engineering presents the most commonly used simulation software, along with the theory involved. It covers chemical engineering thermodynamics, fluid mechanics, material and energy balances, mass transfer operations, reactor design, and computer applications in chemical engineering. Through this book, students learn: What chemical engineers do The functions and theoretical background of basic chemical engineering unit operations How to simulate chemical processes using software packages How to size chemical process units manually and with software How to fit experimental data How to solve linear and nonlinear algebraic equations as well as ordinary differential equations Along with exercises and references, each chapter contains a theoretical description of process units followed by numerous examples that are solved step by step via hand calculations and computer simulation using Hysys/Unisim, PRO/II, Aspen Plus, and SuperPro Designer. Adhering to the Accreditation Board for Engineering and Technology (ABET) criteria, the book gives students the tools needed to solve real problems involving thermodynamics and fluid-phase equilibria, fluid flow, material and energy balances, heat exchangers, reactor design, distillation, absorption, and liquid-liquid extraction.

## **Numerical Methods and Modeling for Chemical Engineers**

### **Computer Methods in Chemical Engineering**

Computational Techniques for Chemical Engineers offers a practical guide to the chemical engineer faced with a problem of computing. The computer is a servant not a master, its value depends on the instructions it is given. This book aims to help the chemical engineer in the right choice of these instructions. The text

begins by outlining the principles of operation of digital and analogue computers and then discussing the difficulties which arise in formulating a problem for solution on such a machine. This is followed by separate chapters on digital computers and their programming; the use of digital computers in chemical engineering design work; optimization techniques and their application in the selection of optimum designs; the solution of sets of non-linear algebraic equations via hill-climbing; and determination of equilibrium compositions by minimization of Gibbs free energy. Subsequent chapters discuss the solution of partial or simultaneous differential equations; parameter estimation in differential equations; continuous systems; and analogue computers.

## **Beyond the Molecular Frontier**

Traditionally, process design and control system design are performed sequentially. It is only recently displayed that a simultaneous approach to the design and control leads to significant economic benefits and improved dynamic performance during plant operation. Extensive research in issues such as 'interactions of design and control', 'analysis and design of plant wide control systems', 'integrated methods for design and control' has resulted in impressive advances and significant new technologies that have enriched the variety of instruments available for the design engineer in her endeavour to design and operate new processes. The field of integrated process design and control has reached a maturity level that mingles the best from process knowledge and understanding and control theory on one side, with the best from numerical analysis and optimisation on the other. Direct implementation of integrated methods should soon become the mainstream design procedure. Within this context 'The Integration of Process Design and Control', bringing together the developments in a variety of topics related to the integrated design and control, will be a real asset for design engineers, practitioners and researchers. Although the individual chapters reach a depth of analysis close to the frontier of current research status, the structure of the book and the autonomous nature of the chapters make the book suitable for a newcomer in the area. The book comprises four distinct parts: Part A: Process characterization and controllability analysis Part B: Integrated process design and control &dashv; Methods Part C: Plant wide interactions of design and control Part D: Integrated process design and control &dashv; Extensions By the end of the book, the reader will have developed a commanding comprehension of the main aspects of integrated design and control, the ability to critically assess the key characteristics and elements related to the interactions between design and control and the capacity to implement the new technology in practice. \* This book brings together the latest developments in a variety of topics related to integrated design and control. \* It is a valuable asset for design engineers, practitioners and researchers. \* The structure of the book and the nature of its chapters also make it suitable for a newcomer to the field.

## **Computational Methods in Chemical Engineering with Maple**

This new volume presents a wealth of practical experience and research on new methodologies and important applications in chemical nanotechnology. It also includes small-scale nanotechnology-related projects that have potential applications in several disciplines of chemistry and nanotechnology. In this book,

contributions range from new methods to novel applications of existing methods to gain understanding of the material and/or structural behavior of new and advanced systems. Topics cover computational methods in chemical engineering and chemoinformatics, studies of some of physico-chemical properties of several important nanoalloy clusters, the use of 3D reconstruction of nanofibrous membranes, nanotechnology research for green engineering and sustainability, nanofiltration and carbon nanotubes applications in water treatment, and much more.

## **Computational Methods for Process Simulation**

Focusing on the application of mathematics to chemical engineering, Applied Mathematical Methods for Chemical Engineers addresses the setup and verification of mathematical models using experimental or other independently derived data. The book provides an introduction to differential equations common to chemical engineering, followed by examples of first-order and linear second-order ordinary differential equations. Later chapters examine Sturm–Liouville problems, Fourier series, integrals, linear partial differential equations, regular perturbation, combination of variables, and numerical methods emphasizing the method of lines with MATLAB® programming examples. Fully revised and updated, this Third Edition: Includes additional examples related to process control, Bessel Functions, and contemporary areas such as drug delivery Introduces examples of variable coefficient Sturm–Liouville problems both in the regular and singular types Demonstrates the use of Euler and modified Euler methods alongside the Runge–Kutta order-four method Inserts more depth on specific applications such as nonhomogeneous cases of separation of variables Adds a section on special types of matrices such as upper- and lower-triangular matrices Presents a justification for Fourier-Bessel series in preference to a complicated proof Incorporates examples related to biomedical engineering applications Illustrates the use of the predictor-corrector method Expands the problem sets of numerous chapters Applied Mathematical Methods for Chemical Engineers, Third Edition uses worked examples to expose several mathematical methods that are essential to solving real-world process engineering problems.

## **Computer Techniques in Chemical Engineering**

Mathematical Methods in Chemical Engineering

## **12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering**

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