Computer Methods In Chemical Engineering Nayef Ghasem

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

Computer Methods in Chemical EngineeringCRC Press

The 18th European Symposium on Computer Aided

Process Engineering contains papers presented at the 18th European Symposium of Computer Aided Process Engineering (ESCAPE 18) held in Lyon, France, from 1-4 June 2008. The ESCAPE series brings the latest innovations and achievements by leading professionals from the industrial and academic communities. The series serves as a forum for engineers, scientists, researchers, managers and students from academia and industry to: - present new computer aided methods, algorithms, techniques related to process and product engineering, - discuss innovative concepts, new challenges, needs and trends in the area of CAPE. This research area bridges fundamental sciences (physics, chemistry, thermodynamics, applied mathematics and computer sciences) with the various aspects of process and product engineering. The special theme for ESCAPE-18 is CAPE for the Users! CAPE systems are to be put in the hands of end users who need functionality and assistance beyond the scientific and technological capacities which are at the core of the systems. The four main topics are: - off-line systems for synthesis and design, - on-line systems for control and operation, - computational and numerical solutions strategies, - integrated and multi-scale modelling and simulation, Two general topics address the impact of CAPE tools and methods on Society and Education. * CD-ROM that accompanies the book contains all research papers and contributions * International in scope with guest speeches and keynote talks from leaders in science and industry * Presents papers covering the latest research, key top areas and

developments in Computer Aided Process Engineering 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

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 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.

While various software packages have become essential for performing unit operations and other kinds of processes in chemical engineering, the fundamental theory and methods of calculation must also be understood to effectively test the validity of these packages and verify the results. Computer Methods in Chemical Engineering, Second Edition presents the most 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. The highly anticipated Second Edition is thoroughly updated to reflect the latest updates in the featured software and has added a focus on real reactors, introduces AVEVA Process Simulation software, and includes new and updated appendixes. Through this book, students will learn the following: 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 calculation 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 chemical engineering students and professionals the tools to solve real problems involving thermodynamics and fluid-phase equilibria, fluid flow, material and energy balances, heat exchangers, reactor design, distillation, absorption, and liquid extraction. This new edition includes many examples simulated by recent software packages. In addition, fluid package information is introduced in correlation to the numerical problems in book. An updated solutions manual and PowerPoint slides are also provided in addition to new video guides and UniSim program files.

In this second edition of An Introduction to Numerical Methods for Chemical Engineers the author has revised text, added new problems, and updated the accompanying computer programs. The result is a text that puts students on the cutting-edge of solving relevant chemical engineering problems.Designed explicitly for undergraduates, this book provides students with software and experience to solve a number of problems.Included in the text are: Numerical algorithms in explicit detail. Example problems from thermodynamic, fluid flow, heat transfer, mass transfer, kinetics, and process design. Equations developed specifically for the student from the example problems. An introduction to advanced numerical techniques, such as finite elements, singular value decomposition, and arc length homotopy.

An introduction to optimization. A systematic approach to process modeling presented with advanced modeling examples. The software that accompanies the book is for IBM-compatible PCs. A solution manual is also available upon request.An Introduction to Numerical Methods for Chemical Engineers was first published in 1988 and has been taught in universities throughout the nation.

This latest edition expands Practical Numerical Methods (PNM) with more VBA to boost Excel's power for modeling and analysis using the same numerical techniques found in specialized math software. Visit the companion web site for more details and additional content: www.d.umn.edu/rdavis/PNM Download the book's Excel and VBA files and learn how to customize your own Excel workbooks: Get the PNMSuite A refined macro-enabled Excel workbook with a suite of over 200 VBA user-defined functions, macros, and user-forms for learning VBA and implementing advanced numerical methods in Excel. Work through the hundreds of examples, illustrations, and animations from the book available in downloadable Excel files that demonstrate applied numerical methods in Excel. Customize the example Excel worksheets and VBA code to tackle your own problems. Try the practice problems for a self-guided study to sharpen your Excel and VBA skills. The first chapter sets up the background for practical problem solving using numerical methods. The next two chapters cover

frequently overlooked features of Excel and VBA for implementing numerical methods in Excel and documenting results. The remaining chapters present powerful numerical techniques using Excel and VBA to find roots to individual and systems of linear and nonlinear equations, evaluate derivatives, perform optimization, model data by regression and interpolation, assess model fidelity, analyze risk and uncertainty, perform integration, and solve ordinary and partial differential equations. This new edition builds on the success of previous editions with 20% new content and updated features in the latest editions of Excel!

The application of modern methods in numerical mathematics on problems in chemical engineering is essential for designing, analyzing and running chemical processes and even entire plants. Scientific Computing in Chemical Engineering II gives the state of the art from the point of view of numerical mathematicians as well as that of engineers. The present volume as part of a two-volume edition covers topics such as the simulation of reactive flows, reaction engineering, reaction diffusion problems, and molecular properties. The volume is aimed at scientists, practitioners and graduate students in chemical engineering, industrial engineering and numerical mathematics.

Modelling in polymer materials science has experienced a dramatic growth in the last two

decades. Advances in modeling methodologies together with rapid growth in computational power have made it possible to address increasingly complex questions both of a fundamental and of a more applied nature. Multiscale Modelling of Polymer Properties assembles research done on modeling of polymeric materials from a hierarchical point of view, in which several methods are combined in a multilevel approach to complex polymeric materials. Contributions from academic and industrial experts are organized in two parts: the first one addresses the methodological aspects while the second one focuses on specific applications. The book aims at comprehensively assessing the current state of the field, including the strengths and shortcomings of available modelling techniques, and at identifying future needs and trends. * Several levels of approximation to the field of polymer modelling; ranging from first-principles to purely macroscopic * Contributions from both academic and industrial experts with varying fields of expertise * Assesses current state of this emerging and rapidly growing field

Contains papers presented at the Third International Symposium on Computer Methods in Biomechanics and Biomedical Engineering (1997), which provide evidence that computer-based models, and in particular numerical methods, are becoming essential tools for the solution of many problems

encountered in the field of biomedical engineering. The range of subject areas presented include the modeling of hip and knee joint replacements, assessment of fatigue damage in cemented hip prostheses, nonlinear analysis of hard and soft tissue, methods for the simulation of bone adaptation, bone reconstruction using implants, and computational techniques to model human impact. Computer Methods in Biomechanics and Biomedical Engineering also details the application of numerical techniques applied to orthodontic treatment together with introducing new methods for modeling and assessing the behavior of dental implants, adhesives, and restorations. For more information, visit the "http://www.uwcm.ac.uk/biorome/international symposium on Computer Methods in Biomechanics and Biomedical Engineering/home page, or "http://www.gbhap.com/Computer_Methods_Biomechanics_Biome dical_Engineering/" the home page for the journal.

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.

Step-by-step instructions enable chemical engineers to masterkey software programs and solve complex problems Today, both students and professionals in chemical engineeringmust solve increasingly complex problems dealing with refineries,fuel cells, microreactors, and pharmaceutical plants, to name afew. With this book as their guide, readers learn to solve theseproblems using their computers and Excel, MATLAB, Aspen Plus, andCOMSOL Multiphysics. Moreover, they learn how to check theirsolutions and validate their results to make sure they have solvedthe problems correctly. Now in its Second Edition, Introduction to ChemicalEngineering Computing is based on the author's firsthandteaching experience. As a result, the emphasis is on problemsolving. Simple introductions help readers become conversant witheach program and then tackle a broad range of problems in chemicalengineering, 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, andexamples to guide readers through all the programs and types ofchemical engineering problems. Problems at the end of each chapter,ranging from simple to difficult, allow readers to gradually buildtheir skills, whether they solve the problems themselves or inteams. In

addition, the book's accompanying website lists thecore principles learned from each problem, both from a chemicalengineering and a computational perspective. Covering a broad range of disciplines and problems withinchemical engineering, Introduction to Chemical EngineeringComputing is recommended for both undergraduate and graduatestudents as well as practicing engineers who want to know how tochoose the right computer software program and tackle almost anychemical engineering problem.

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.

This book provides in-depth knowledge to solve engineering, geometrical, mathematical, and scientific problems with the help of advanced computational methods with a focus on mechanical and materials engineering. Divided into three subsections covering design and fluids, thermal engineering and materials engineering, each chapter includes exhaustive literature review along with thorough analysis and future research scope. Major topics covered pertains to computational fluid dynamics, mechanical performance, design, and fabrication including wide range of applications in industries as automotive, aviation, electronics,

nuclear and so forth. Covers computational methods in design and fluid dynamics with a focus on computational fluid dynamics Explains advanced material applications and manufacturing in labs using novel alloys and introduces properties in material Discusses fabrication of graphene reinforced magnesium metal matrix for orthopedic applications Illustrates simulation and optimization gear transmission, heat sink and heat exchangers application Provides unique problem-solution approach including solutions, methodology, experimental setup, and results validation This book is aimed at researchers, graduate students in mechanical engineering, computer fluid dynamics,fluid mechanics, computer modeling, machine parts, and mechatronics.

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.

Chemistry and chemical engineering have changed significantly in the last decade. They have broadened their scopeâ€"into biology, nanotechnology, materials science, computation, and advanced methods of process systems engineering and controlâ€"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 sciencesâ€"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.

Chemical Engineering Computation with MATLAB®, Second Edition continues to present basic to advanced levels of problem-solving techniques using MATLAB as the computation environment. The Second Edition provides even more examples and problems extracted from core chemical engineering subject areas and all code is updated to MATLAB version 2020. It also includes a new chapter on computational intelligence and: Offers exercises and extensive problem-solving instruction and solutions for various problems Features solutions developed using fundamental principles to construct mathematical models and an equation-oriented approach to generate numerical results Delivers a wealth of examples to 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 Includes an appendix offering an introduction to MATLAB for readers unfamiliar with the program, which will allow them to write their own MATLAB programs and follow the examples in the book 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 This essential textbook readies engineering students, researchers, and professionals to be proficient in the use of MATLAB to solve sophisticated real-world problems within the interdisciplinary field of chemical engineering. The text features a solutions manual, lecture slides, and MATLAB program files._

30th European Symposium on Computer Aided Chemical Engineering, Volume 47 contains the papers presented at the 30th European Symposium of Computer Aided Process

Engineering (ESCAPE) event held in Milan, Italy, May 24-27, 2020. It is a valuable resource for chemical engineers, chemical process engineers, researchers in industry and academia, students, and consultants for chemical industries. Presents findings and discussions from the 30th European Symposium of Computer Aided Process Engineering (ESCAPE) event Offers a valuable resource for chemical engineers, chemical process engineers, researchers in industry and academia, students, and consultants for chemical industries

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.

CAMD or Computer Aided Molecular Design refers to the design of molecules with desirable properties. That is, through CAMD, one determines molecules that match a specified set of (target) properties. CAMD as a technique has a very large potential as in principle, all kinds of chemical, bio-chemical and material products can be designed through this technique. This book mainly deals with macroscopic properties and therefore does not cover molecular design of large, complex chemicals such as drugs. While books have been written on computer aided molecular design relating to drugs and large complex chemicals, a book on systematic formulation of CAMD problems and solutions, with emphasis on theory and practice, which helps one to learn, understand and apply the technique is currently unavailable. · This title brings together the theoretical aspects related to Computer Aided Molecular Design, the different techniques that have been developed and the different applications that have been reported. · Contributing authors are among the leading

researchers and users of CAMD · First book available giving a systematic formulation of CAMD problems and solutions Computer aided process engineering (CAPE) plays a key design and operations role in the process industries. This conference features presentations by CAPE specialists and addresses strategic planning, supply chain issues and the increasingly important area of sustainability audits. Experts collectively highlight the need for CAPE practitioners to embrace the three components of sustainable development: environmental, social and economic progress and the role of systematic and sophisticated CAPE tools in delivering these goals.

The European Symposium on Computer Aided Process Engineering (ESCAPE) series presents the latest innovations and achievements of leading professionals from the industrial and academic communities. The ESCAPE series serves as a forum for engineers, scientists, researchers, managers and students to present and discuss progress being made in the area of Computer Aided Process Engineering (CAPE). European industries large and small are bringing innovations into our lives, whether in the form of new technologies to address environmental problems, new products to make our homes more comfortable and energy efficient or new therapies to improve the health and well-being of European citizens. Moreover, the European Industry needs to undertake research and technological initiatives in response to humanity's "Grand Challenges", described in the declaration of Lund, namely, Global Warming, Tightening Supplies of Energy, Water and Food, Ageing Societies, Public Health, Pandemics and Security. Thus, the Technical Theme of ESCAPE 21 will be "Process Systems Approaches for Addressing Grand Challenges in Energy, Environment, Health, Bioprocessing & Nanotechnologies".

This book covers a variety of topics in mechanics, with a

special emphasis to fluid mechanics and energy transfer. Chapters are based on selected contributions presented during the Algerian Congress of Mechanics (CAM 2017), held on November 26 - 30, 2017, in Constantine, Algeria. The book covers theoretical analysis, modeling, and numerical treatment of performance-related problems of new refrigeration systems, heating and cooling. It reports on experimental research to solve problems related to the flow of microfluids, and relevant applications in the areas of chemical engineering, biochemistry, biomedicine and renewable energy. Further topics include methods for maintenance of mechanical structures, strength, wear, fracture, damage and life of structures, and image processing solutions for the design and 3D manufacturing of mechanical parts. Improvement, control and regulation of urban road traffic are also discussed in this book, thus offering a comprehensive, practice-oriented reference guide for academics and professionals.

"A companion book including interactive software for students and professional engineers who want to utilize problem-solving software to effectively and efficiently obtain solutions to realistic and complex problems. An Invaluable reference book that discusses and Illustrates practical numerical problem solving in the core subject areas of Chemical Engineering. Problem Solving in Chemical Engineering with Numerical Methods provides an extensive selection of problems that require numerical solutions from throughout the core subject areas of chemical engineering. Many are completely solved or partially solved using POLYMATH as the representative mathematical problem-solving software, Ten representative problems are also solved by Excel, Maple, Mathcad, MATLAB, and Mathematica. All problems are clearly organized and all necessary data are provided. Key equations are presented or derived. Practical aspects of

efficient and effective numerical problem solving are emphasized. Many complete solutions are provided within the text and on the CD-ROM for use in problem-solving exercises."--BOOK JACKET.Title Summary field provided by Blackwell North America, Inc. All Rights Reserved

Computer Methods and Recent Advances in Geomechanics contains the proceedings (abstracts book 472 pages + full paper USB-drive 2052 pages) of the 14th International Conference of the International Association for Computer Methods and Advances in Geomechanics (Kyoto, Japan, 22-25 September, 2014). The contributions cover computer methods, material m

The proceedings of the fourth symposium on this topic examine the rapid advances and innovations being made in the theoretical and applied aspects of structural masonry. Focusing on the integration of computer modelling with experimental methods, assessment techniques, restoration and retro-fitting procedures, this is a thorough examination of the subject by leading international experts. Contains numerous graphs and tables.

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.

This book deals with finite element analysis of structures and will be of value to students of civil, structural and mechanical engineering at final year undergraduate and post-graduate level. Practising structural engineers and researchers will also find it useful. Authoritative and up-to-date, it provides a thorough grounding in matrix-tensor analysis and the underlying theory, and a logical development of its application to structures.

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.

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.

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

Substantially revised and updated, Computer Methods for Engineering with MATLAB® Applications, Second Edition presents equations to describe engineering processes and systems. It includes computer methods for solving these equations and discusses the nature and validity of the numerical results for a variety of engineering problems. This edition now uses MATLAB in its discussions of computer solution. New to the Second Edition Recent advances in computational software and hardware A large number of MATLAB commands and programs for solving exercises and to encourage students to develop their own computer programs for specific problems Additional exercises and examples in all chapters New and updated references The text follows a systematic approach for obtaining physically realistic, valid, and accurate results through numerical modeling. It employs examples from many engineering areas to explain the elements involved in the numerical solution and make the presentation relevant and interesting. It also incorporates a wealth of solved exercises to supplement the discussion and illustrate the ideas and methods presented. The book shows how a computational approach can provide physical insight and obtain inputs for the analysis and design of practical engineering systems.

Mathematical Modelling of Gas-Phase Complex

Reaction Systems: Pyrolysis and Combustion, Volume 45, gives an overview of the different steps involved in the development and application of detailed kinetic mechanisms, mainly relating to pyrolysis and combustion processes. The book is divided into two parts that cover the chemistry and kinetic models and then the numerical and statistical methods. It offers a comprehensive coverage of the theory and tools needed, along with the steps necessary for practical and industrial applications. Details thermochemical properties and "ab initio" calculations of elementary reaction rates Details kinetic mechanisms of pyrolysis and combustion processes Explains experimental data for improving reaction models and for kinetic mechanisms assessment Describes surrogate fuels and molecular reconstruction of hydrocarbon liquid mixtures Describes pollutant formation in combustion systems Solves and validates the kinetic mechanisms using numerical and statistical methods Outlines optimal design of industrial burners and optimization and dynamic control of pyrolysis furnaces Outlines large eddy simulation of turbulent reacting flows

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.

Applications of numerical mathematics and scientific computing to chemical engineering.