Chemical Thermodynamics For Process Simulation

Introduction to Chemical Engineering Computing
Chemical Thermodynamics for Process Simulation
Process Analysis and Simulation in Chemical Engineering
Chemical Engineering Computation with MATLAB®
Introductory Chemical Engineering Thermodynamics
Addressing the Gap between Studies and Chemical Industry
A Practical Guide Using a Three Steps Methodology
Chemical Thermodynamics for Process Simulation
Phase Equilibrium Engineering
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Computer-Aided Case Studies
Process Modelling and Simulation with Finite Element Methods
The Benefit of Mathematical Methods in Applications of the Chemical Industry
Using Aspen Plus in Thermodynamics Instruction
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The Importance of Thermodynamics on Process Simulation Modeling
Computer Methods in Chemical Engineering
A TEXTBOOK OF CHEMICAL ENGINEERING THERMODYNAMICS
Distillation
Chemical & Process Thermodynamics
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Chemical Thermodynamics
A Step-by-Step Guide
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Principles and Practice
Modeling of Chemical Kinetics and Reactor Design
From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design
Advanced Process Control and Simulation for Chemical Engineers
Simulation of Industrial Processes for Control Engineers
A Step-by-Step Guide
Select Thermodynamic Models for Process Simulation
Industrial Chemical Process Analysis and Design
Theory and Applications

GREGORY PALOMA

Introduction to Chemical Engineering Computing CRC Press
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 Thermodynamics for Process Simulation John Wiley & Sons
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Process Analysis and Simulation in Chemical Engineering Walter de Gruyter GmbH & Co KG
A Practical, Up-to-Date Introduction to Applied Thermodynamics, Including Coverage of Process Simulation Models and an Introduction to Biological Systems Introductory Chemical Engineering Thermodynamics, Second Edition, helps readers master the fundamentals of applied thermodynamics as practiced today: with extensive development of molecular perspectives that enables adaptation to fields including biological systems, environmental applications, and nanotechnology. This text is distinctive in making molecular perspectives accessible at the introductory level and connecting properties with practical implications. Features of the second edition include Hierarchical instruction with increasing levels of detail: Content requiring deeper levels of theory is clearly delineated in separate sections and chapters Early introduction to the overall perspective of composite systems like distillation

columns, reactive processes, and biological systems Learning objectives, problem-solving strategies for energy balances and phase equilibria, chapter summaries, and “important equations” for every chapter Extensive practical examples, especially coverage of non-ideal mixtures, which include water contamination via hydrocarbons, polymer blending/recycling, oxygenated fuels, hydrogen bonding, osmotic pressure, electrolyte solutions, zwitterions and biological molecules, and other contemporary issues Supporting software in formats for both MATLAB® and spreadsheets Online supplemental sections and resources including instructor slides, ConcepTests, coursecast videos, and other useful resources

Chemical Engineering Computation with MATLAB® John Wiley & Sons

The only textbook that applies thermodynamics to real-world process engineering problems This must-read for advanced students and professionals alike is the first book to demonstrate how chemical thermodynamics work in the real world by applying them to actual engineering examples. It also discusses the advantages and disadvantages of the particular models and procedures, and explains the most important models that are applied in process industry. All the topics are illustrated with examples that are closely related to practical process simulation problems. At the end of each chapter, additional calculation examples are given to enable readers to extend their comprehension. Chemical Thermodynamics for Process Simulation instructs on the behavior of fluids for pure fluids, describing the main types of equations of state and their abilities. It discusses the various quantities of interest in process simulation, their correlation, and prediction in detail. Chapters look at the important terms for the description of the thermodynamics of mixtures; the most important models and routes for phase equilibrium calculation; models which are applicable to a wide variety of non-electrolyte systems; membrane processes; polymer thermodynamics; enthalpy of reaction; chemical equilibria, and more. -Explains thermodynamic fundamentals used in process simulation with solved examples -Includes new chapters about modern measurement techniques, retrograde condensation, and simultaneous description of chemical equilibrium -Comprises numerous solved examples, which simplify the understanding of the often complex calculation procedures, and discusses advantages and disadvantages of models and procedures -Includes estimation methods for thermophysical properties and phase equilibria thermodynamics of alternative separation processes -Supplemented with MathCAD-sheets and DDBST programs for readers to reproduce the examples Chemical Thermodynamics for Process Simulation is an ideal resource for those working in the fields of process development, process synthesis, or process optimization, and an excellent book for students in the engineering sciences.

Introductory Chemical Engineering

Thermodynamics PHI Learning Pvt. Ltd.
Process Control: Modeling, Design, and Simulation is the first complete introduction to process control that fully integrates software tools-helping you master critical techniques hands-on, using MATLAB-based computer simulations. Author B. Wayne Bequette includes process control diagrams, dynamic modeling, feedback control, frequency response analysis techniques, control loop tuning, and start-to-finish chemical process control case studies.
Addressing the Gap between Studies and Chemical Industry John Wiley & Sons
The only textbook that applies thermodynamics to real-world process engineering problems This must-read for advanced students and professionals alike is the first book to demonstrate how chemical thermodynamics work in the real world by applying them to actual engineering examples. It also discusses the advantages and disadvantages of the particular models and procedures, and explains the most important models that are applied in process industry. All the topics are illustrated with examples that are closely related to practical process simulation problems. At the end of each chapter, additional calculation examples are given to enable readers to extend their comprehension. Chemical Thermodynamics for Process Simulation instructs on the behavior of fluids for pure fluids, describing the main types of equations of state and their abilities. It discusses the various quantities of interest in process simulation, their correlation, and prediction in detail. Chapters look at the important terms for the description of the thermodynamics of mixtures; the most important models and routes for phase equilibrium calculation; models which are applicable to a wide variety of non-electrolyte systems; membrane processes; polymer thermodynamics; enthalpy of reaction; chemical equilibria, and more. -Explains thermodynamic fundamentals used in process simulation with solved examples -Includes new chapters about modern measurement techniques, retrograde condensation, and simultaneous description of chemical equilibrium - Comprises numerous solved examples, which simplify the understanding of the often complex calculation procedures, and discusses advantages and disadvantages of models and procedures -Includes estimation methods for thermophysical properties and phase equilibria thermodynamics of alternative separation processes -Supplemented with MathCAD-sheets and DDBST programs for readers to reproduce the examples Chemical Thermodynamics for Process Simulation is an ideal resource for those working in the fields of process development, process synthesis, or process optimization, and an excellent book for students in the engineering sciences.
A Practical Guide Using a Three Steps Methodology Elsevier
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.

Chemical Thermodynamics for Process Simulation

Elsevier

Selecting the best type of reactor for any particular chemical reaction, taking into consideration safety, hazard analysis, scale-up, and many other factors is essential to any industrial problem. An understanding of chemical reaction kinetics and the design of chemical reactors is key to the success of the of the chemist and the chemical engineer in such an endeavor. This valuable reference volume conveys a basic understanding of chemical reactor design methodologies, incorporating control, hazard analysis, and other topics not covered in similar texts. In addition to covering fluid mixing, the treatment of wastewater, and chemical reactor modeling, the author includes sections on safety in chemical reaction and scale-up, two topics that are often neglected or overlooked. As a real-world introduction to the modeling of chemical kinetics and reactor design, the author includes a case study on ammonia synthesis that is integrated throughout the text. The text also features an accompanying CD, which contains computer programs developed to solve modeling problems using numerical methods. Students, chemists, technologists, and chemical engineers will all benefit from this comprehensive volume. Shows readers how to select the best reactor design, hazard analysis,

and safety in design methodology Features computer programs developed to solve modeling problems using numerical methods
Phase Equilibrium Engineering Cengage Learning
Applications in Design and Simulation of Sustainable Chemical Processes addresses the challenging applications in designing eco-friendly but efficient chemical processes, including recent advances in chemistry and catalysis that rely on renewable raw materials. Grounded in the fundamental knowledge of chemistry, thermodynamics, chemical reaction engineering and unit operations, this book is an indispensable resource for developing and designing innovating chemical processes by employing computer simulations as an efficient conceptual tool. Targeted to graduate and post graduate students in chemical engineering, as well as to professionals, the book aims to advance their skills in process innovation and conceptual design. The work completes the book Integrated Design and Simulation of Chemical Processes by Elsevier (2014) authored by the same team. Includes comprehensive case studies of innovative processes based on renewable raw materials Outlines Process Systems Engineering approach with emphasis on systematic design methods Employs steady-state and dynamic process simulation as problem analysis and flowsheet creation tool Applies modern concepts, as process integration and intensification, for enhancing the sustainability
COSMO-RS Elsevier
Industrial Chemical Process Analysis and Design uses chemical engineering principles to explain the transformation of basic raw materials into major chemical products. The book discusses traditional processes to create products like nitric acid, sulphuric acid, ammonia, and methanol, as well as more novel products like bioethanol and biodiesel. Historical perspectives show how current chemical processes have developed over years or even decades to improve their yields, from the discovery of the chemical reaction or physico-chemical principle to the industrial process needed to yield commercial quantities. Starting with an introduction to process design, optimization, and safety, Martin then provides stand-alone chapters—in a case study fashion—for commercially important chemical production processes. Computational software tools like MATLAB®, Excel, and Chemcad are used throughout to aid process analysis. Integrates principles of chemical engineering, unit operations, and chemical reactor engineering to understand process synthesis and analysis Combines traditional computation and modern software tools to compare different solutions for the same problem Includes historical perspectives and traces the improving efficiencies of commercially important chemical production processes Features worked examples and end-of-chapter problems with solutions to show the application of concepts discussed in the text
Computer-Aided Case Studies John Wiley & Sons
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.

Process Modelling and Simulation with Finite Element Methods Prentice Hall

As the chemical process industry is among the most energy demanding sectors, chemical engineers are endeavoring to contribute towards sustainable future. Due to the limitation of fossil fuels, the need for energy independence, as well as the environmental problem of the greenhouse gas effect, there is a large increasing interest in the research and development of chemical processes that require less capital investment and reduced operating costs and lead to high eco-efficiency. The use of heat pumps is a hot topic due to many advantages, such as low energy requirements as well as an increasing number of industrial applications. Therefore, in the current book, authors are focusing on use of heat pumps in the chemical industry, providing an overview of heat pump technology as applied in the chemical process industry, covering both theoretical and practical aspects: working principle, applied thermodynamics, theoretical background, numerical examples and case studies, as well as practical applications. The worked-out examples have been included to instruct students, engineers and process designers about how to design various heat pumps used in the industry. Reader friendly resources namely relevant equations, diagrams, figures and references that reflect the current and upcoming heat pump technologies, will be of great help to all readers from the chemical and petrochemical industry, biorefineries and other related areas.

The Benefit of Mathematical Methods in Applications of the Chemical Industry

Editions TECHNIP

The selection of the most adequate thermodynamic model in a process simulation is an issue that most process engineer has to face sooner or later. This book, conceived as a practical guide, aims at providing adequate answers by analysing the questions to be looked at. The analysis (first chapter) yields three keys that are further discussed in three different chapters. (1) A good understanding of the properties required in the process, and their method of calculation is the first key. The second chapter provides to that end in a synthetic manner the most important equations that are derived from the fundamental principes of thermodynamics. (2) An adequate description of the mixture, which is a combination of models and parameters, is the second key. The third chapter makes the link

between components and models, both from a numerical (parameterisation) and physical (molecular interactions) point of view. Finally, (3) a correct view of the phase behaviour and trends in regard of the process conditions is the third key. The fourth chapter illustrates the phase behaviour and makes model recommendations for the most significant industrial systems. A decision tree is provided at the end of this chapter. In the last chapter, the key questions are reviewed for a number of typical processes. This book is intended for process engineers, who are not specialists of thermodynamics but are confronted with this kind of problems and need a reference book, as well as process engineering students who will find an original approach to thermodynamics, complementary of traditional lectures

Using Aspen Plus in Thermodynamics Instruction Springer

This book offers a modern view of process control in the context of today's technology. It provides innovative chapters on the growth of educational, scientific, and industrial research among chemical engineers. It presents experimental data on thermodynamics and provides a broad understanding of the main computational techniques used for chemical processing. Readers will gain an understanding of the areas of process control that all chemical engineers need to know. The information is presented in a concise and readable format. The information covers the basics and also provides unique topics, such as using a unified approach to model representations, statistical quality control, and model-based control. The methods presented have been successfully applied in industry to solve real problems. Designed as an advanced research guide in process dynamics and control, the book will be useful in chemical engineering courses as well as for the teaching of mechanical, nuclear, industrial, and metallurgical engineering.

Modeling and Simulation of Chemical Process Systems Elsevier

Phase equilibrium knowledge is required for the design of all sorts of chemical processes that may involve separations, reactions, fluids flow, particle micronization, etc. Indeed, different phase behavior scenarios are required for a rational conceptual process design. The aim of this chapter is to present the possible fluid mixture phase behavior that can be found in binary, ternary, and multicomponent systems. Moreover, representation of phase behavior in terms of phase diagrams is discussed. Dealing with phase diagrams of complex mixtures is not an easy task for beginners; however, very simple concepts are behind the rules for their construction. Phase diagrams are essential tools for phase equilibrium engineering as they provide valuable hints to understand the process and to assess the feasible and optimum operating regions. In this chapter, the "phenomenological" meaning of each phase behavior and its relation with molecular properties is discussed. A special attention is given to binary system phase behavior. Even though, in practice we rarely found such simple mixtures, they furnish a great deal of information for the understanding of multicomponent systems.

Using Aspen Plus in

Thermodynamics Instruction Chemical Thermodynamics for Process Simulation
A step-by-step guide for students (and faculty) on the use of Aspen in teaching thermodynamics • Easily-accessible modern computational techniques opening up new vistas in teaching thermodynamics A range of applications of Aspen Plus in the prediction and calculation of thermodynamic properties and phase behavior using the state-of-the art methods • Encourages students to develop engineering insight by doing repetitive calculations with changes in parameters and/or models • Calculations and application examples in a step-by-step manner designed for out-of-classroom self-study • Makes it possible to easily integrate Aspen Plus into thermodynamics courses without using in-class time • Stresses the application of thermodynamics to real problems
The Importance of Thermodynamics on Process Simulation Modeling World Scientific 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 Engineering Elsevier Inc. Chapters
In recent years remarkable progress has been made applying mathematical methods in process simulation and optimization, resulting in significant improvements in the design and operation of industrial production plants. Simulation and Optimization in Process Engineering: The Benefit of Mathematical Methods in Applications of the Process Industry brings together examples where the successful transfer of progress made in mathematical simulation and optimization has led to innovations in an industrial context that created substantial benefit. Containing introductory accounts on scientific progress in the most relevant topics of process engineering (substance properties, simulation, optimization, optimal control and real time optimization), the examples included illustrate how such

scientific progress has been transferred to innovations that delivered a measurable impact, covering details of the methods used, how they were implemented in an industrial context, which hurdles had to be overcome and how they created benefit - often beyond what had first been expected. With each chapter bringing together expertise from academia and industry, this book is the first of its kind, providing demonstratable insights. Recent mathematical methods are transformed into industrially relevant innovations Covers recent progress in mathematical simulation and optimization in a process engineering context with chapters written by experts in both academia and industry Provides insight into industrially relevant challenges in a digitized world

A TEXTBOOK OF CHEMICAL ENGINEERING THERMODYNAMICS Elsevier

This book presents a systematic description and case studies of chemical engineering modelling and simulation based on the MATLAB/FEMLAB tools, in support of selected topics in undergraduate and postgraduate programmes that require numerical solution of complex balance equations (ordinary differential equations, partial differential equations, nonlinear equations, integro-differential equations). These systems arise naturally in analysis of transport phenomena, process systems, chemical reactions and chemical thermodynamics, and particle rate processes. Templates are given for modelling both state-of-the-art research topics (e.g. microfluidic networks, film drying, multiphase flow, population balance equations) and case studies of commonplace design calculations -- mixed phase reactor design, heat transfer, flowsheet analysis of unit operations, flash distillations, etc. The great strength of this book is that it makes modelling and simulating in the MATLAB/FEMLAB environment approachable to both the novice and the expert modeller.

Distillation John Wiley & Sons

Computer simulation is the key to comprehending and controlling the full-scale industrial plant used in the chemical, oil, gas and electrical power industries. Simulation of Industrial Processes for Control Engineers shows how to use the laws of physics and chemistry to produce the equations to simulate dynamically all the most important unit operations found in process and power plant. The book explains how to model chemical reactors, nuclear reactors, distillation columns, boilers, deaerators, refrigeration vessels, storage vessels for liquids and gases, liquid and gas flow through pipes and pipe networks, liquid and gas flow through installed control valves, control valve dynamics (including nonlinear effects such as static friction), oil and gas pipelines, heat exchangers, steam and gas turbines, compressors and pumps, as well as process controllers (including three methods of integral desaturation). The phenomenon of markedly different time responses ("stiffness") is considered and various ways are presented to get around the potential problem of slow execution time. The book demonstrates how linearization may be used

to give a diverse check on the correctness of the as-programmed model and explains how formal techniques of model validation may be used to produce a quantitative check on the simulation model's overall validity. The material is based on many years' experience of modelling and simulation in the chemical and power industries, supplemented in recent years by university teaching at the undergraduate and postgraduate level. Several important new results are presented. The depth is sufficient to allow real industrial problems to be solved, thus making the book attractive to engineers working in industry. But the book's step-by-step approach makes the text appropriate also for post-graduate students of control engineering and for undergraduate students in electrical, mechanical and chemical engineering who are studying process control in their second year or later.