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Chemical Process Design, Simulation and Optimization
 Process Modeling and Simulation for Chemical Engineers
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 Ludwig's Applied Process Design for Chemical and Petrochemical Plants
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Chemical Process Design, Simulation and Optimization Elsevier
 Computer aided process engineering (CAPE) tools have been very successfully used in process design and product engineering for a long time. In particular, simulation and modelling tools have enabled engineers to analyse and understand the behaviour of selected processes prior to building actual plants. The aim of design or retrofit of chemical processes is to produce profitably products that satisfy the societal needs, ensuring safe and reliable operation of each process, as well as minimising any effects on the environment. This involves the conceptual design or retrofit of plants and processes, novel manufacturing approaches, process/control system design interactions and operability, manufacturability, environmental and safety issues. Backed by current studies, this 2-volume set gives a comprehensive survey of the various approaches and latest developments on the use of CAPE in the process industry. An invaluable reference to the scientific and industrial community in

the field of computer aided process and product engineering.

Process Modeling and Simulation for Chemical Engineers
 John Wiley & Sons

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.

Process Modeling and Simulation for Chemical Engineers CRC Press

This book provides a rigorous treatment of the fundamental concepts and techniques involved in process modeling and simulation. The book allows the reader to: (i) Get a solid grasp of "under-the-hood" mathematical results (ii) Develop models of sophisticated processes (iii) Transform models to different geometries and domains as appropriate (iv) Utilize various model simplification techniques (v) Learn simple and effective computational methods for model simulation (vi) Intensify the effectiveness of their research

Modeling and Simulation for Chemical Engineers: Theory and Practice begins with an introduction to the terminology of process modeling and simulation. Chapters 2 and 3 cover fundamental and constitutive relations, while Chapter 4 on model formulation builds on these relations. Chapters 5 and 6 introduce the advanced techniques of model transformation and simplification. Chapter 7 deals with model simulation, and the final chapter reviews important mathematical concepts. Presented in a methodical, systematic way, this book is suitable as a self-study guide or as a graduate reference, and includes examples, schematics and diagrams to enrich understanding. End of chapter problems (with solutions and computer software available online) are designed to further stimulate readers to apply the newly-learned concepts. End of chapter problems (with solutions and computer software available online) are designed to further stimulate readers to apply the newly learned concepts.

Computational Methods for Process Simulation Springer

The Fourth Edition of *Applied Process Design for Chemical and Petrochemical Plants Volume 2* builds upon the late Ernest E. Ludwig's classic chemical engineering process design manual. Volume Two focuses on distillation and packed towers, and presents the methods and fundamentals of plant design along with supplemental mechanical and related data, nomographs, data charts and heuristics. The Fourth Edition is significantly expanded and updated, with new topics that ensure readers can analyze problems and find practical design methods and solutions to accomplish their process design objectives. A true application-driven book, providing clarity and easy access to essential process plant data and design information. Covers a complete range of basic day-to-day petrochemical operation topics. Extensively revised with new material on distillation process performance; complex-mixture fractionating, gas processing, dehydration, hydrocarbon absorption and stripping; enhanced distillation types

Chemical Process Design and Integration Elsevier

The use of simulation plays a vital part in developing an integrated approach to process design. By helping save time and money before the actual trial of a concept, this practice can assist with troubleshooting, design, control, revamping, and more. *Process Modelling and Simulation in Chemical, Biochemical and Environmental Engineering* explores effective modeling and simulation approaches for solving equations. Using a systematic treatment of model development and simulation studies for chemical, biochemical, and environmental processes, this book explains the simplification of a complicated process at various levels with the help of a "model sketch." It introduces several types of models, examines how they are developed, and provides examples from a wide range of applications. This includes the simple models based on simple laws such as Fick's law, models that consist of generalized equations such as equations of motion, discrete-event models and stochastic models (which consider at least one variable as a discrete variable), and models based on population balance. Divided into 11 chapters, this book: Presents a systematic approach of model development in view of the simulation need. Includes modeling techniques to model hydrodynamics, mass and heat transfer, and reactors for single

as well as multi-phase systems. Provides stochastic and population balance models. Covers the application and development of artificial neural network models and hybrid ANN models. Highlights gradients based techniques as well as statistical techniques for model validation and sensitivity analysis. Contains examples on development of analytical, stochastic, numerical, and ANN-based models and simulation studies using them. Illustrates modeling concepts with a wide spectrum of classical as well as recent research papers. *Process Modelling and Simulation in Chemical, Biochemical and Environmental Engineering* includes recent trends in modeling and simulation, e.g. artificial neural network (ANN)-based models, and hybrid models. It contains a chapter on flowsheeting and batch processes using commercial/open source software for simulation.

Chemical Engineering Process Simulation Butterworth-Heinemann

Tools for Chemical Product Design: From Consumer Products to Biomedicine describes the challenges involved in systematic product design across a variety of industries and provides a comprehensive overview of mathematical tools aimed at the design of chemical products, from molecular design to customer products. Chemical product design has become increasingly important over the past decade and includes a wide range of sectors including gasoline additives and blends in the petroleum industry, active ingredients and excipients in the pharmaceutical industry, and a variety of consumer products and specialty chemicals. Traditionally, such products have been designed through trial and error methods, which not only are time-consuming, but more importantly only provide limited knowledge that can be translated into next generation products. Features an impressive collection of contributions from leading researchers in the field. Presents the latest tools available across a variety of industries. Describes the challenges involved in systematic product design as well as the latest methods for solving such problems. Covers a wide range of sectors including gasoline additives and blends in the petroleum industry, active ingredients and excipients in the pharmaceutical industry, and a variety of consumer products and specialty chemicals.

Software Architectures and Tools for Computer Aided Process Engineering Wiley-Interscience

This book presents a theoretical analysis of the modern methods used for modeling various chemical engineering processes. Currently, the two primary problems in the chemical industry are the optimal design of new devices and the optimal control of active processes. Both of these problems are often solved by developing new methods of modeling. These methods for modeling specific processes may be different, but in all cases, they bring the mathematical description closer to the real processes by using appropriate experimental data. In this book, the authors detail a new approach for the modeling of chemical processes in column apparatuses. Further, they describe the types of neural networks that have been shown to be effective in solving important chemical engineering problems. Readers are also presented with mathematical models of integrated bioethanol supply chains (IBSC) that achieve improved economic and environmental sustainability. The integration of energy and mass processes is one of the most powerful tools for creating sustainable and energy efficient production systems. This book defines the main approaches for the thermal integration of periodic processes, direct and indirect, and the recent integration of small-scale solar thermal dryers with phase change materials as energy accumulators. An exciting overview of new approaches for the modeling of chemical engineering processes, this book serves as a guide for the important innovations being made in theoretical chemical engineering.

Step-Growth Polymerization Process Modeling and Product Design Gulf Professional Publishing

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

Modeling Chemical Processes in Materials John Wiley & Sons
Chemical Engineering Process Simulation, Second Edition guides users through chemical processes and unit operations using the main simulation software used in the industrial sector. The book helps predict the characteristics of a process using mathematical models and computer-aided process simulation tools, as well as how to model and simulate process performance before detailed process design takes place. Content coverage includes steady-state and dynamic simulation, process design, control and optimization. In addition, readers will learn about the simulation of natural gas, biochemical, wastewater treatment and batch processes. Provides an updated and expanded new edition that contains 60-70% new content Guides readers through chemical processes and unit operations using the primary simulation software used in the industrial sector Covers the fundamentals of process simulation, theory and advanced applications Includes case studies of various difficulty levels for practice and for applying developed skills Features step-by-step guides to using UniSim Design, SuperPro Designer, Symmetry, Aspen HYSYS and Aspen Plus for process simulation novices

Integrated Design and Simulation of Chemical Processes Elsevier
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 Mathematical and Physical Modeling of Materials Processing Operations Springer Nature

Understand quantitative model step-growth polymerization plans and how to predict properties of the product polymer with the essential information in Step-Growth Polymerization Process Modeling and Product Design. If you want to learn how to simulate step-growth polymerization processes using commercial software and seek an in-depth, quantitative understanding of how to develop, use, and deploy these simulations, consult this must-have guide. The book focuses on quantitative relationships between key process input variables (KPIVs) and key process output variables (KPOVs), and the integrated modeling of an entire polymer manufacturing train.

Computer Aided Process and Product Engineering (CAPE) CRC Press

A comprehensive and example oriented text for the study of chemical process design and simulation Chemical Process Design and Simulation is an accessible guide that offers information on the most important principles of chemical engineering design and includes illustrative examples of their application that uses simulation software. A comprehensive and practical resource, the text uses both Aspen Plus and Aspen Hysys simulation software. The author describes the basic methodologies for computer aided design and offers a description of the basic steps of process simulation in Aspen Plus and Aspen Hysys. The text reviews the design and simulation of individual simple unit operations that includes a mathematical model of each unit operation such as reactors, separators, and heat exchangers. The author also explores the design of new plants and simulation of existing plants where conventional chemicals and material mixtures with measurable compositions are used. In addition, to aid in comprehension, solutions to examples of real problems are included. The final section covers plant design and simulation of processes using nonconventional components. This important resource: Includes information on the application of both the Aspen Plus and Aspen Hysys software that enables a comparison of the two software systems Combines the basic theoretical principles of chemical process and design with real-world examples Covers both processes with conventional organic chemicals and processes with more complex materials such as solids, oil blends, polymers and electrolytes Presents examples that are solved using a new version of Aspen software, ASPEN One 9 Written for students and academics in the field of process design, Chemical Process Design and Simulation is a practical and accessible guide to the chemical process design and simulation using proven software.

Tools For Chemical Product Design CRC Press

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.

Process Modelling and Simulation in Chemical, Biochemical and Environmental Engineering John Wiley & Sons

Since process models are nowadays ubiquitous in many applications, the challenges and alternatives related to their development, validation, and efficient use have become more apparent. In addition, the massive amounts of both offline and online data available today open the door for new applications and solutions. However, transforming data into useful models and information in the context of the process industry or of bio-systems requires specific approaches and considerations such as new modelling methodologies incorporating the complex, stochastic, hybrid and distributed nature of many processes in particular. The same can be said about the tools and software environments used to describe, code, and solve such models for their further exploitation. Going well beyond mere simulation tools, these advanced tools offer a software suite built around the models, facilitating tasks such as experiment design, parameter estimation, model initialization, validation, analysis, size reduction, discretization, optimization, distributed computation, co-simulation, etc. This Special Issue collects novel developments in these topics in order to address the challenges brought by the use of models in their different facets, and to reflect state of the art developments in methods, tools and industrial applications. *Introduction to Software for Chemical Engineers, Second Edition* CRC Press

A New Approach to HAZOP of Complex Chemical Processes provides practical methods to identify and categorize chemical process complexities systematically. The book follows a holistic assessment of risks and required safeguards which enables readers to define the boundaries of HAZOP 4.0 accurately. The book is written by authors who have decades of experience in advanced process monitoring and artificial intelligence to support HAZOP teams with a holistic dynamic simulation and multivariable monitoring of the complex systems, and to assess historical failure and accident data and information using artificial intelligence techniques in a user-friendly way. Presents complexity assessment and management to the conventional HAZOP ? Provides multivariable monitoring to dynamic simulation for a holistic hazard identification and process safeguards requirements ? Describes AI to support the HAZOP team with code-based requirements and historical failure and accident data ? Explains AI to find the dynamic behavior of process based on empirical data without the models with simplification assumptions

Molecular Modeling Techniques in Material Sciences Elsevier
In this valuable volume, new and original research on various topics on chemical engineering and technology is presented on modeling and simulation, material synthesis, wastewater treatment, analytical techniques, and microreactors. The research presented here can be applied to technology in food, paper and pulp, polymers, petrochemicals, surface coatings, oil technology aspects, among other uses. The book is divided into five sections: modeling and simulation environmental applications materials and applications processes and applications analytical methods Topics include: modeling and simulation of chemical processes process integration and intensification separation processes advances in unit operations and processes chemical reaction engineering fuel and energy advanced materials CFD and transport processes wastewater treatment The valuable research presented here will be of interest to researchers, scientists, industry practitioners, as well as upper-level students.

Chemical Process Engineering, Volume 2 LAP Lambert Academic

Publishing

Increasingly useful in materials research and development, molecular modeling is a method that combines computational chemistry techniques with graphics visualization for simulating and predicting the structure, chemical processes, and properties of materials. *Molecular Modeling Techniques in Materials Science* explores the impact of using molecular modeling for various simulations in industrial settings. It provides an overview of commonly used methods in atomistic simulation of a broad range of materials, including oxides, superconductors, semiconductors, zeolites, glass, and nanomaterials. The book presents information on how to handle different materials and how to choose an appropriate modeling method or combination of techniques to better predict material behavior and pinpoint effective solutions. Discussing the advantages and disadvantages of various approaches, the authors develop a framework for identifying objectives, defining design parameters, measuring accuracy/accounting for error, validating and assessing various data collected, supporting software needs, and other requirements for planning a modeling project. The book integrates the remarkable developments in computation, such as advanced graphics and faster, cheaper workstations and PCs with new advances in theoretical techniques and numerical algorithms. *Molecular Modeling Techniques in Materials Science* presents the background and tools for chemists and physicists to perform in-silico experiments to understand relationships between the properties of materials and the underlying atomic structure. These insights result in more accurate data for designing application-specific materials that withstand real process conditions, including hot temperatures and high pressures.

A Step by Step Approach to the Modeling of Chemical Engineering Processes National Academies Press

CHEMICAL PROCESS ENGINEERING Written by one of the most prolific and respected chemical engineers in the world and his co-author, also a well-known and respected engineer, this two-volume set is the "new standard" in the industry, offering engineers and students alike the most up-to-date, comprehensive, and state-of-the-art coverage of processes and best practices in the field today. This new two-volume set explores and describes integrating new tools for engineering education and practice for better utilization of the existing knowledge on process design. Useful not only for students, university professors, and practitioners, especially process, chemical, mechanical and metallurgical engineers, it is also a valuable reference for other engineers, consultants, technicians and scientists concerned about various aspects of industrial design. The text can be considered as complementary to process design for senior and graduate students as well as a hands-on reference work or refresher for engineers at entry level. The contents of the book can also be taught in intensive workshops in the oil, gas, petrochemical, biochemical and process industries. The book provides a detailed description and hands-on experience on process design in chemical engineering, and it is an integrated text that focuses on practical design with new tools, such as Microsoft Excel spreadsheets and UniSim simulation software. Written by two of the industry's most trustworthy and well-known authors, this book is the new standard in chemical, biochemical, pharmaceutical, petrochemical and petroleum refining. Covering design, analysis, simulation, integration, and, perhaps most importantly, the practical application of Microsoft Excel-UniSim software, this is the most comprehensive and up-to-date coverage of all of the latest developments in the industry. It is a must-have for any engineer or student's library.

Ludwig's Applied Process Design for Chemical and Petrochemical Plants John Wiley & Sons

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.

Industrial Chemical Process Analysis and Design Elsevier

ASPEN PLUS® Comprehensive resource covering Aspen Plus V12.1 and demonstrating how to implement the program in versatile chemical process industries Aspen Plus®: Chemical Engineering Applications facilitates the process of learning and later mastering Aspen Plus®, the market-leading chemical process modeling software, with step-by-step examples and succinct explanations. The text enables readers to identify solutions to various process engineering problems via screenshots of the Aspen Plus® platforms in parallel with the related text. To aid in information retention, the text includes end-of-chapter problems and term project problems, online exam and quiz problems for instructors that are parametrized (i.e., adjustable) so that each student will have a standalone version, and extra online material for students, such as Aspen Plus®-related files, that are used in the working tutorials throughout the entire textbook. The second edition of Aspen Plus®: Chemical Engineering Applications includes information on: Various new features that were embedded into Aspen Plus V12.1 and existing features which have been modified Aspen Custom Modeler (ACM), covering basic features to show how to merge customized models into Aspen Plus simulator New updates to process dynamics and control and process economic analysis since the first edition was published Vital areas of interest in relation to the software, such as polymerization, drug solubility, solids handling, safety measures, and energy saving For chemical engineering students and industry professionals, the second edition of Aspen Plus®: Chemical Engineering Applications is a key resource for understanding Aspen Plus and the new features that were added in version 12.1 of the software. Many supplementary learning resources help aid the reader with information retention.

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