Process Flowsheeting

This publication brings together the latest research findings in the key area of chemical process control; including dynamic modelling and simulation - modelling and model validation for application in linear and nonlinear model-based control: nonlinear model-based predictive control and optimization - to facilitate constrained real-time optimization of chemical processes; statistical control techniques - major developments in the statistical interpretation of measured data to guide future research; knowledge-based v model-based control - the integration of theoretical aspects of control and optimization theory with more recent developments in artificial intelligence and computer science.

Chemical Process Structures and Information Flows focuses on the role of computers in the understanding of chemical processes, including the use of simulation and optimization in computational problems. The book first underscores graphs and digraphs and pipeline networks. Discussions focus on cutsets and connectivity, directed graphs, trees and circuits, matrix representation of digraphs and graphs, reachability matrix, alternative problem formulations and specifications, and steady state conditions in cyclic networks. The manuscript also ponders on computation sequence in process flowsheet calculations and sparse matrix computation. The publication examines scheduling and design of batch plants, including scheduling of products and operations, characteristics of batch processes, branch and bound methods, and multipurpose batch plants. The text also elaborates on observability and redundancy and process data reconciliation and rectification. The manuscript is a valuable reference for chemical engineering students and readers interested in chemical processes and information flow.

Frontal Algorithms for Equation-based Chemical Process Flowsheeting on Vector and Parallel Computers

Commemorative Issue to Celebrate the Life and Work of Prof. Roger W.H. Sargent

Computational Experiments in Equation-based Chemical Process Flowsheeting

On Sparse Pivoting Strategies for Chemical Process Flowsheeting

Numerical Studies in Equation-based Chemical Process Flowsheeting

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

Second International Conference on Chemical Engineering Education presents the situation in chemical engineering education in Germany, Hungary, Spain, Japan, and in the United States. This book depicts an awareness of the problems of professional education together with a wide spectrum of opinions on their solution. Organized into 39 chapters, this book begins with an overview of the actual situation of chemical engineering education program in Spain. This text then examines the detailed formalities of chemical engineering in secondary schools. Other chapters consider the change in chemical engineering education in Japan due to the change of chemical industries as well as by a great change of students' attitude. This book discusses as well the curriculum proposal for the education of undergraduate and graduate levels as well as foreign students' education. The final chapter reviews the European situation of chemical engineering education system. This book is a valuable resource for teachers and students of chemical engineering.

Application of Computer Graphics to Process Flowsheeting

Introduction to Software for Chemical Engineers

Process Systems Engineering for Biofuels Development

A Strategy for Simulation and Optimization of Process Flowsheets

Technologies and Applications

Methodological Analysis of Equation-oriented Process FlowsheetingProcess FlowsheetingCambridge University Press

Two packages of subroutines were developed to perform material balances on chemical processes using the simultaneous modular approach and the equation-based approach. The performances of these packages were compared for five different processes under at least two conditions: one with no design specifications, and one with two or more design specifications. The equations arising from chemical process simulation using the simultaneous modular approach and equation-based approach are nonlinear. Therefore, two subroutines were developed to solve systems of nonlinear equations using a modification of Powell's dogleg method as proposed by Chen and Stadtherr. One of the nonlinear solver subroutines uses sparse matrix techniques and updates the Jacobian through Schubert's formula. The other uses full matrix techniques and the Jacobian is updated through Broyden's formula. Both subroutines were tested with five problems and the results compared. The results obtained with the two packages of subroutines and the nonlinear solver subroutines compared well with similar

problems from the open literature.

Visualizing Industrial Multivariable Control Constraints in Operations and Chemical Process Flowsheeting in MATLAB

Second International Conference on Chemical Engineering Education

A Three-Day Symposium Organised by the Institution of Chemical Engineers on Behalf of the European Federation of Chemical Engineers, Co-Sponsored by the American Institute of Chemical Engineers and the Society of Chemical Engineers, Japan, and Held at Rob

Product-Driven Process Design

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._

This book offers a comprehensive coverage of process simulation and flowsheeting, useful for undergraduate students of Chemical Engineering and Process Engineering as theoretical and practical support in Process Design, Process Simulation, Process Engineering, Plant Design, and Process Control courses. The main concepts related to process simulation and application tools are presented and discussed in the framework of typical problems found in engineering design. The topics presented in the chapters are organized in an inductive way, starting from the more simplistic simulations up to some complex problems.

Process Flowsheeting of a Hybrid Nickel Leach Circuit

Two-pass Strategies for Sparse Matrix Computations in Chemical Process Flowsheeting Problems

the Aspen project

Advanced Control of Chemical Processes 1994

Chemical Engineering Computation with MATLAB®

Proceedings of the 3rd International Seminar, held in Lyon, May 25-27, 1983

Product-driven process design - from molecule to enterprise provides process engineers and process engineering students with access to a modern and stimulating methodology to process and product design. Throughout the book the links between product design and process design become evident while the reader is guided step-by-step through the different stages of the intertwining product and process design activities. Both molecular and enterprise-wide considerations in design are introduced and addressed in detail. Several examples and case studies in emerging areas such as bio- and food-systems, pharmaceuticals and energy are discussed and presented. This book is an excellent guide and companion for undergraduate, graduate students as well as professional practitioners.

Methodological Analysis of Equation-oriented Process Flowsheeting

Use of Iterative Linear Solvers in Process Flowsheeting Simulations

Computational Strategies for Chemical Process Flowsheeting and Optimization

Studies on the Dynamics of Equation-based Chemical Process Flowsheeting Systems

Design and Development of Process Flowsheeting and Synthesis System for the Design of Energy Efficient Processes Using Spreadsheet Programs

The book will highlight major trends and developments in the field of microbial fuels, with contributions from a number of highly experienced researchers. It will serve as a comprehensive reference for industrial stakeholders, scientists, researchers and graduate students interested in microbial fuels. The aims of this work are to present the technologies and perspectives taking into account different socio-economical contexts. A specific chapter will focus on the general perspectives of microbial fuels for low-income and emerging countries.

The field of chemical engineering is in constant evolution, and access to information technology is changing the way chemical engineering problems are addressed. Inspired by the need for a user-friendly chemical engineering text that demonstrates the real-world applicability of different computer programs, Introduction to Software for Chemical Engineers acquaints readers with the capabilities of various general purpose, mathematical, process modeling and simulation, optimization, and specialized software packages, while explaining how to use the software to solve typical problems in fluid mechanics, heat and mass transfer, mass and energy balances, unit operations, reactor engineering, and process and equipment design and control. Employing nitric acid production, methanol and ammonia recycle loops, and SO2 oxidation reactor case studies and other practical examples, Introduction to Software for Chemical Engineers shows how computer packages such as Excel, MATLAB®, Mathcad, CHEMCAD, Aspen HYSYS®, gPROMS, CFD, DEM, GAMS, and AIMMS are used in the design and operation of chemical reactors, distillation columns, cooling towers, and more. Make Introduction to Software for Chemical Engineers your go-to guide and quick reference for the use of computer software in chemical engineering applications.

An Implementation of the Simultaneous-modular Method for Process Flowsheeting and Optimization

Integrated Design and Simulation of Chemical Processes
Hydrogen as an Energy Carrier
Process Flowsheeting
On Applying Vector Computers to Chemical Process Flowsheeting

ICT Innovations for Sustainability is an investigation of how information and communication technology can contribute to sustainable development. It presents clear definitions of sustainability, suggesting conceptual frameworks for the positive and negative effects of ICT on sustainable development. It reviews methods of assessing the direct and indirect impact of ICT systems on energy and materials demand, and examines the results of such assessments. In addition, it investigates ICT-based approaches to supporting sustainable patterns of production and consumption, analyzing them at various levels of abstraction – from end-user devices, Internet infrastructure, user behavior, and social practices to macro-economic indicators. Combining approaches from Computer Science, Information Systems, Human-Computer Interaction, Economics, and Environmental Sciences, the book presents a new, holistic perspective on ICT for Sustainability (ICT4S). It is an indispensable resource for anyone working in the area of ICT for Energy Efficiency, Life Cycle Assessment of ICT, Green IT, Green Information Systems, Environmental Informatics, Energy Informatics, Sustainable HCI, or Computational Sustainability.

We present several frontal algorithms for solving the large, sparse, linear equation systems arising in equation-based (EB) chemical process flowsheeting. The frontal approach is generally used as a banded matrix solver in connection with finite element problems. We adapt it here to the more general process flowsheeting matrix. The motivation is that the frontal approach exploits vector computer architectures by treating parts of the sparse flowsheeting matrix as full submatrices, thereby allowing arithmetic operations to be performed with full-matrix code (without indirect addressing). On parallel computers, the inner loops of the elimination phase can be multitasked by simply subdividing the frontal matrix. Flowsheeting results show that the frontal approach performs very well on the CRAY X-MP/416 architecture. However, several pivot steps have to be overlapped on the CRAY-2 computer to ensure that both vector floating-point pipes are kept busy. Results concerning the use of multiple pivot steps indicate that two new assembly-language kernels designed for the CRAY-2 computer prove to be very efficient for performing rank-two and rank-four updates. In fact, the multitasked implementations of these kernels can achieve computational rates well over 1 Gigaflop when used as the nucleus of a frontal solver for EB flowsheeting. Overall, the frontal codes perform very well in comparison to the general sparse code,

LU1SOL, and shows considerable promise for the solution of EB flowsheeting matrices on supercomputers. The solution of large, sparse linear equation systems is also a critical phase of the simultaneous solution of interlinked distillation columns. If the modeling equations for a distillation system are grouped by plate, the linear systems take on an almost-block-tridiagonal structure. We apply here the frontal approach to solve these almost-banded linear systems on vector computers. Results for nine interlinked systems show that the frontal approach is up to an order of magnitude faster than the general sparse code, LU1SOL, on the CRAY X-MP computer and is between one and two orders of magnitude faster than LU1SOL on the CDC Cyber 175.

Chemical Process Structures and Information Flows

Process Analysis and Simulation in Chemical Engineering

Computer-aided industrial process design

Equation-based Chemical Process Flowsheeting and Optimization

Microbial Fuels

Much work has already been carried out on the High Pressure Acid Leaching (HPAL) and Atmospheric Leaching (AL) of laterite in various acidic solutions. However, much of this data is scattered and discrete. As such, there is a gap between the generation of experimental data and the utilisation of this data to optimise the operation of a flowsheet. The steps followed during the course of this work involved first the experimental identification of rheology/kinetics of laterite. An operational, flexible, steady-state model of a hybrid pressure acid leaching circuits was then developed to take into account the effect of different operating parameters and calculate the major operating costs, i.e acid and steam consumption. With the aid of the model, the performance of nickel circuits was analysed and the optimum operating parameters identified.

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".

ICT Innovations for Sustainability

From Molecule to Enterprise
21st European Symposium on Computer Aided Process Engineering
Process Engineering
Strategies for Process Flowsheeting

The mathematical modeling of the transient behavior of a complex chemical process naturally leads to the formulation of large sets of Differential and Algebraic equations (DAEs). The very flexible and effective equation-based (EB) approach in dynamic process flowsheeting calls for the simultaneous solution of the DAE set. However the numerical solution of DAEs is not trivial. The convergence properties of the numerical methods used for solving DAE systems depend upon a very important and peculiar property of a DAE, its index. Problems of index higher than two cannot be adequately handled by existing DAE codes and are practically unsolvable. It was shown that the index is affected by, among other factors, the choice of design variables and equations. Since these choices are often made rather arbitrarily, an important conclusion is that the index should be a criterion in making this choice. An algorithm was presented for selecting design equations and variables to ensure the formation of an index-one DAE. Furthermore alternative index-reducing formulations for incorporating design variables in the DAE model were shown to be possible. Strategies were presented for predicting the overall flowsheet index given the indices of single units, or groups of units, and the topology of the flowsheet. As a result, the formidable task of estimating the entire flowsheet index becomes more manageable since it can be dealt with on a smaller scale. The strategy proposed first partitions the flowsheet into groups of units to be considered together for their index identification. The information obtained from the application of the partitioning algorithm is subsequently combined with the results of the index analysis on integrated two-unit systems to obtain the particular flowsheet index. The proposed strategy was evaluated by applying it to a number of test problems representing relatively complex flowsheets. The insight that was gained from the index analysis was applied toward the development of a new EB dynamic process flowsheeting package, DSEQUEL-II. This package was successfully used for the simulation of flowsheeting problems, some involving process control schemes, of size up to several hundred variables. A number of computational issues was also studied toward the development of a truly robust and efficient dynamic simulator.

Process flowsheeting concerns the use of computers to stimulate and design chemical plant of all types, such as petroleum refineries, petrochemical complexes or even food factories. In this 1979 introduction to the topic the authors examine the role of flowsheeting

in process plant design and look at the various techniques on which computer-aided systems may be based. For each one of these approaches the advantages and disadvantages are clearly stated and the four most important methods are described in detail. In each case the motivation for its development is analysed and its use is illustrated by a number of practical examples. Particular attention is devoted to the underlying technology of process flowsheeting systems, and an introduction to the analysis of degrees of freedom in flowsheeting and a guide to further reading are also included. This book will still hold value for those interested in the historical development of process flowsheeting.

Efficient Use of Thermodynamic Data in Process Flowsheeting

This book celebrates the life, work and influence of Professor Roger W.H. Sargent of Imperial College London. It does so through a range of original contributions that span the wide academic and industry interests of Professor Sargent. Roger Sargent passed away in late 2018, but his legacy lives on through his enormous academic tree, which traces to the early 1960s. That huge body of work has also had significant impacts on industrial practices. Roger was regarded as "the father of Process Systems Engineering (PSE)". This area of Chemical Engineering continues to influence the modelling, design, control, optimization and integrated performance of industrial and related processes. This book highlights some of those impacts and the ongoing importance of PSE in helping to solve some of the grand challenges of our time.

A comprehensive overview of current developments and applications in biofuels production Process Systems Engineering for Biofuels Development brings together the latest and most cutting-edge research on the production of biofuels. As the first book specifically devoted to process systems engineering for the production of biofuels, Process Systems Engineering for Biofuels Development covers theoretical, computational and experimental issues in biofuels process engineering. Written for researchers and postgraduate students working on biomass conversion and sustainable process design, as well as industrial practitioners and engineers involved in process design, modeling and optimization, this book is an indispensable guide to the newest developments in areas including: Enzyme-catalyzed biodiesel production Process analysis of biodiesel production (including kinetic modeling, simulation and optimization) The use of ultrasonification in biodiesel production Thermochemical processes for biomass transformation to biofuels Production of alternative biofuels In addition to the comprehensive overview of the subject of biofuels found in the Introduction of the book, the authors of various chapters have provided extensive discussions of the production and separation of biofuels via novel applications and techniques.