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Mathematical Modeling and Scale-up of Liquid Chromatography



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Mathematical Modeling And Scaleup Of Liquid Chromatography

**Gunter Jagschies, Gail K. Sofer, Lars
Hagel**



Mathematical Modeling And Scaleup Of Liquid Chromatography:

Mathematical Modeling and Scale-up of Liquid Chromatography Tingyue Gu, 2012-12-06 Liquid chromatography has proved to be one of the most important tools for separations. Rapid development in biotechnology has increased the demand for chromatography in analytical, preparative and large scale applications. The understanding of the dynamics of chromatography is imperative for the scale up. This book is a systematic treatment of the general rate models for various forms of liquid chromatography including adsorption, size exclusion, affinity, reversed phase, hydrophobic interaction and radial flow chromatography. Thermodynamic and mass transfer effects in liquid chromatography are discussed. Applications of computer programs for the rate models are described and the procedures for the scale up of preparative and large scale liquid chromatography using the general rate models are given.

Mathematical Modeling and Scale-Up of Liquid Chromatography Tingyue Gu, 2015-04-06 Tingyue Gu's second edition provides a comprehensive set of nonlinear multicomponent liquid chromatography (LC) models for various forms of LC such as adsorption, size exclusion, ion exchange, reversed phase, affinity, isocratic, gradient elution and axial radial flow LC. Much has advanced since the first edition of this book and the author's software described here is now used for teaching and research in 32 different countries. This book comes together with a complete software package with graphical user interface for personal computers offered free for academic applications. Additionally, this book provides detailed methods for parameter estimation of mass transfer coefficients, bed voidage, particle porosity and isotherms. The author gives examples of how to use the software for predictions and scale up. In contrast to the first edition, authors do not need to deal with complicated math. Instead, they focus on how to obtain a few parameters for simulation and how to compare simulation results with experimental data. After reading the detailed descriptions in the book, a reader is able to use the simulation software to investigate chromatographic behavior without doing actual experiments. This book is aimed at readers who are interested in learning about LC behaviors and at those who want to scale up LC for preparative and large scale applications. Both academic personnel and industrial practitioners can benefit from the use of the book. This new edition includes new models and software for pellicular cored beads in liquid chromatography. Introduction of user friendly software with graphical user interface. Detailed descriptions on how to use the software. Step by step instructions on parameter estimation for the models. New mass transfer correlations for parameter estimation. Experimental methods for parameter estimation. Several actual examples using the model for product development and scale up. Updated literature review.

Mathematical Modeling and Scale-Up of Liquid Chromatography Tingyue Gu, 2015 Tingyue Gu's second edition provides a comprehensive set of nonlinear multicomponent liquid chromatography (LC) models for various forms of LC such as adsorption, size exclusion, ion exchange, reversed phase, affinity, isocratic, gradient elution and axial radial flow LC. Much has advanced since the first edition of this book and the author's software described here is now used for teaching and research in 32 different countries. This book comes together

with a complete software package with graphical user interface for personal computers offered free for academic applications. Additionally, this book provides detailed methods for parameter estimation of mass transfer coefficients, bed voidage, particle porosity, and isotherms. The author gives examples of how to use the software for predictions and scale up. In contrast to the first edition, authors do not need to deal with complicated math. Instead, they focus on how to obtain a few parameters for simulation and how to compare simulation results with experimental data. After reading the detailed descriptions in the book, a reader is able to use the simulation software to investigate chromatographic behavior without doing actual experiments. This book is aimed at readers who are interested in learning about LC behaviors and at those who want to scale up LC for preparative and large scale applications. Both academic personnel and industrial practitioners can benefit from the use of the book. This new edition includes:

- New models and software for pellicular cored beads in liquid chromatography
- Introduction of user friendly software with graphical user interface
- Detailed descriptions on how to use the software
- Step by step instructions on parameter estimation for the models
- New mass transfer correlations for parameter estimation
- Experimental methods for parameter estimation
- Several actual examples using the model for product development and scale up
- Updated literature review

Modeling of Process Intensification Frerich J. Keil, 2007-04-09

Combining the knowledge involved in process engineering and process modeling, this is the first book to cover all modeling methods applicable to process intensification. Both the editors and authors are renowned experts from industry and academia in the various fields of process modeling and integrated chemical processes. Following an introduction to the topic, the book goes on to look at equipment and operational methods: monolithic catalysis, HEX, micro and reverse flow reactors, catalytic and reactive distillation, the simulated moving bed, and vibration bubble column, as well as ultrasound and ultrasonic reactors. A final chapter is devoted to processes under supercritical conditions. In its treatment of hot topics of multidisciplinary interest, this book is of great value to researchers and engineers alike.

Handbook of Process Chromatography Gunter Jagschies, Gail K. Sofer, Lars Hagel, 2007-12-08

This book will update the original edition published in 1997. Since the publication of the first edition, the biotechnology and biologics industries have gained extensive knowledge and experience in downstream processing using chromatography and other technologies associated with recovery and purification unit operations. This book will tie that experience together for the next generation of readers. Updates include:

- sources and productivity types of products made today
- experiences in clinical and licensed products
- economics
- current status of validation
- illustrations and tables
- automated column packing
- automated systems

New topics include:

- the use of disposables
- multiproduct versus dedicated production
- design principles for chromatography media and filters
- ultrafiltration principles
- and optimization
- risk assessments
- characterization studies
- design space
- platform technologies
- process analytical technologies
- PATs
- biogenerics
- comparability assessments

Key Features: new approaches to process optimization, use of platform technologies, applying risk assessment to process design.

Principles and Practice of Modern Chromatographic

Methods Kevin Robards, Danielle Ryan, 2021-12-03 Principles and Practice of Modern Chromatographic Methods Second Edition takes a comprehensive unified approach in its presentation of chromatographic techniques Like the first edition the book provides a scientifically rigid but easy to follow presentation of chromatography concepts that begins with the purpose and intent of chromatographic theory the what and why that are left out of other books attempting to cover these principles This fully revised second edition brings the content up to date covering recent developments in several new sections and an additional chapter on composite methods New topics include sample profiling sample preparation sustainable green chemistry 2D chromatography miniaturization nano LC HILIC and more Contains thorough chapters that begin with an updated schematic overview and a visual representation of the content Avoids the obfuscation of different terminologies and classification systems that are prevalent in the area such as the relationship between liquid chromatography and column chromatography Provides integrated and comprehensive topic coverage based on chromatographic bibliometrics and survey reports on the relative usage of chromatographic techniques

Preparative Chromatography for Separation of Proteins Arne Staby, Anurag S. Rathore, Satinder Ahuja, 2017-03-06 Preparative Chromatography for Separation of Proteins addresses a wide range of modeling techniques strategies and case studies of industrial separation of proteins and peptides Covers broad aspects of preparative chromatography with a unique combination of academic and industrial perspectives Presents Combines modeling with compliance using of Quality by Design QbD approaches including modeling Features a variety of chromatographic case studies not readily accessible to the general public Represents an essential reference resource for academic industrial and pharmaceutical researchers Preparative Chromatography H.

Schmidt-Traub, 2006-03-06 This interdisciplinary approach combines the chemistry and engineering involved to describe the conception and improvement of chromatographic processes The book covers recent developments in preparative chromatographic processes for the separation of smaller molecules using standard laboratory equipment as well as the detailed conception of industrial chemical plants Following an introductory section on the history of chromatography the current state of research and the design of chromatographic processes the book goes on to define the general terminology There then follow sections on solid materials and packed columns process concepts Final chapters on modeling and determination of model parameters the design and optimization of preparative chromatographic processes and chromatographic reactors allow for the optimum selection of chromatographic systems Essential for chemists and engineers working in the chemicals and pharmaceutical industries as well as for food technologies due to the interdisciplinary nature of these processes Process Modeling, Simulation, and Environmental Applications in Chemical Engineering Bharat A.

Bhanvase, Rajendra P. Ugwekar, 2016-10-14 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

Design, Simulation and Optimization of Adsorptive and Chromatographic Separations: A Hands-On Approach Kevin R. Wood, Y. A. Liu, Yueying Yu, 2018-02-27 A comprehensive resource to the construction use and modification of the wide variety of adsorptive and chromatographic separations Design Simulation and Optimization of Adsorptive and Chromatographic Separations offers the information needed to effectively design simulate and optimize adsorptive and chromatographic separations for a wide range of industrial applications The authors noted experts in the field cover the fundamental principles the applications and a range of modeling techniques for the processes The text presents a unified approach that includes the ideal and intermediate equations and offers a wealth of hands on case studies that employ the rigorous simulation packages Aspen Adsorption and Aspen Chromatography The text reviews the effective design strategies details design considerations and the assumptions which the modelers are allowed to make The authors also cover shortcut design methods as well as mathematical tools that help to determine optimal operating conditions This important text Covers everything from the underlying phenomena to model optimization and the customization of model code Includes practical tutorials that allow for independent review and study Offers a comprehensive review of the construction use and modification of the wide variety of adsorptive and chromatographic separations Contains contributions from three noted experts in the field Written for chromatographers process engineers chemists and other professionals Design Simulation and Optimization of Adsorptive and Chromatographic Separations offers a comprehensive review of the construction use and modification of adsorptive and chromatographic separations

Bioprocess and Analytics Development for Virus-based Advanced Therapeutics and Medicinal Products (ATMPs) Saurabh Gautam, Abhilash I. Chiramel, Roland Pach, 2023-08-10 This book reviews the knowledge methods and available techniques in the rapidly advancing field of virus based vaccines and gene therapeutics It also highlights new innovative tools and interdisciplinary techniques for bioprocess development and analytics of viruses and viral vectors As such it provides a timely and highly relevant resource since current advances in pharmaceutical research have seen the rise of vaccines and advanced therapeutics and medicinal products ATMPs that rely on the power of viruses However developing bioprocesses and analytics required to create this often called magic bullet i e gene therapy remains an extremely challenging and costly task This book offers strategies for overcoming hurdles and difficulties within in all the necessary steps of viral vector development from scalability to purification methods and quality control The book is intended for researchers working in academia or industry

as well as graduate students pursuing a career in virology Bioseparations Science and Engineering Roger G. Harrison, Paul W. Todd, Scott R. Rudge, Demetri P. Petrides, 2015-01-27 Designed for undergraduates graduate students and industry practitioners Bioseparations Science and Engineering fills a critical need in the field of bioseparations Current comprehensive and concise it covers bioseparations unit operations in unprecedented depth In each of the chapters the authors use a consistent method of explaining unit operations starting with a qualitative description noting the significance and general application of the unit operation They then illustrate the scientific application of the operation develop the required mathematical theory and finally describe the applications of the theory in engineering practice with an emphasis on design and scaleup Unique to this text is a chapter dedicated to bioseparations process design and economics in which a process simulator SuperPro Designer is used to analyze and evaluate the production of three important biological products New to this second edition are updated discussions of moment analysis computer simulation membrane chromatography and evaporation among others as well as revised problem sets Unique features include basic information about bioproducts and engineering analysis and a chapter with bioseparations laboratory exercises Bioseparations Science and Engineering is ideal for students and professionals working in or studying bioseparations and is the premier text in the field **Experiment and Modelling of the Competitive Sorption and Transport of Chlorinated Ethenes in Porous Media** Manuel Alejandro Salas Avila, 2005 **European Symposium on Computer Aided Process Engineering - 10** Sauro Pierucci, 2000-05-10 This book includes papers presented at ESCAPE 10 the 10th European Symposium on Computer Aided Process Engineering held in Florence Italy 7-10th May 2000 The scientific program reflected two complementary strategic objectives of the Computer Aided Process Engineering CAPE Working Party one checked the status of historically consolidated topics by means of their industrial application and their emerging issues while the other was addressed to opening new windows to the CAPE audience by inviting adjacent Working Parties to co operate in the creation of the technical program The former CAPE strategic objective was covered by the topics Numerical Methods Process Design and Synthesis Dynamics Control Process Modeling Simulation and Optimization The latter CAPE strategic objective derived from the European Federation of Chemical Engineering EFCE promotion of scientific activities which autonomously and transversely work across the Working Parties terms of references These activities enhance the exchange of the know how and knowledge acquired by different Working Parties in homologous fields They also aim to discover complementary facets useful to the dissemination of tools and of novel procedures As a consequence the Working Parties Environmental Protection Loss Prevention and Safety Promotion and Multiphase Fluid Flow were invited to assist in the organization of sessions in the area of A Process Integrated Approach for Environmental Benefit Loss Prevention and Safety Computational Fluid Dynamics A total of 473 abstracts from all over the world were evaluated by the International Scientific Committee Out of them 197 have been finally selected for the presentation and reported into this book Their authors come from thirty different countries The selection of the papers was

carried out by twenty eight international reviewers These proceedings will be a major reference document to the scientific and industrial community and will contribute to the progress in Computer Aided Process Engineering

Lattice Boltzmann Modeling for Chemical Engineering ,2020-06-19 Lattice Boltzmann Modeling for Chemical Engineering Volume 56 in the Advances in Chemical Engineering series highlights new advances in the field with this new volume presenting interesting chapters on Simulations of homogeneous and heterogeneous chemical reactions LBM for 3D Chemical Reactors LBM Simulations of PEM fuel cells LBM for separation processes LBM for two phase flow bio reactors and more Provides the authority and expertise of leading contributors from an international board of authors Presents the latest release in the Advances in Chemical Engineering series Includes the latest information on Lattice Boltzmann Modeling for Chemical Engineering

Engineering and Food for the 21st Century Jorge Weltri-Chanes,Jose Miguel Aguilera,2002-03-25 Engineering and Food for the 21st Century presents important reviews and up to date discussions of major topics relating to engineering and food Internationally renowned contributors discuss a broad base of food engineering and related subjects including research and prospective industrial applications

Comprehensive Biotechnology ,2011-08-26 The second edition of Comprehensive Biotechnology Six Volume Set continues the tradition of the first inclusive work on this dynamic field with up to date and essential entries on the principles and practice of biotechnology The integration of the latest relevant science and industry practice with fundamental biotechnology concepts is presented with entries from internationally recognized world leaders in their given fields With two volumes covering basic fundamentals and four volumes of applications from environmental biotechnology and safety to medical biotechnology and healthcare this work serves the needs of newcomers as well as established experts combining the latest relevant science and industry practice in a manageable format It is a multi authored work written by experts and vetted by a prestigious advisory board and group of volume editors who are biotechnology innovators and educators with international influence All six volumes are published at the same time not as a series this is not a conventional encyclopedia but a symbiotic integration of brief articles on established topics and longer chapters on new emerging areas Hyperlinks provide sources of extensive additional related information material authored and edited by world renown experts in all aspects of the broad multidisciplinary field of biotechnology Scope and nature of the work are vetted by a prestigious International Advisory Board including three Nobel laureates Each article carries a glossary and a professional summary of the authors indicating their appropriate credentials An extensive index for the entire publication gives a complete list of the many topics treated in the increasingly expanding field

Computer Applications in Biotechnology 2004 Marie-Noelle Pons,Jan Van Impe,2005-08-02

Separations Chemistry Fedor Macášek,James D. Navratil,2016-06-06 Separation of chemical species is a gate to final success of synthesis and preparation of compounds in pure and defined state Variability of natural and artificial mixtures to be treated is enormous Task of chemistry is to separate components of homogeneous mixtures the gaseous and liquid solutions The book concentrates on understanding the basic

philosophies of both equilibrium and nonequilibrium chemical thermodynamics and engineering performance that lay in principle of separation technique such as distillation crystallization centrifugation sorption membrane separations chromatography and liquid liquid extraction Specific phenomena connected with photochemical separation isotope composition and radioactivity are discussed as well The book is written for advanced students of chemistry having the knowledge of physical chemistry Calculation examples are based on the international system of units Unique list of over 1 300 full references covers scientific literature of the eighteenth to the twenty first centuries Microorganisms to Combat Pollution E. Rosenberg, 2012-12-06 This volume contains material first presented at an international workshop on the Use of Microorganisms to Combat Pollution held in Israel May 10 18 1992 The workshop was sponsored by the Bat Sheva de Rothschild Foundation for the Advancement of Science and included microbiologists biochemists and geneticists from universities environmental agencies and the military Each of the contributors to this volume is an acknowledged expert on the treatment of one or more types of pollution using microorganisms or their enzymes This book differs from most published symposia proceedings in the breadth of coverage of each subject Most of the chapters are divided into three parts a A general presentation of the source and toxicity of the pollutant b a review of the current state of the science on the biodegradation of that pollutant and c the authors unique research experiences on the problem In several examples the authors have presented data from both laboratory studies and field trials Thus the book contains not only the theoretical background on the biodegradation of pollutants but also practical experiences in applying this knowledge to solving significant pollution problems

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