# Computational Models For Polydisperse Particulate And Multiphase Systems

Addressing all aspects of the design, modeling and simulation of chromatographic processes, this result-oriented primer provides a practical guide to all the necessary approaches, methodologies and tools. Beginning with key definitions and concepts, it builds up from the most simple to the most complex situations, including multicomponent systems, non-uniform velocity profiles, bed instability, particle size distributions, and the influence of complex environments on chromatographic process design. In addition to covering classical approaches, it introduces efficient tools for investigating chromatographic processes, such as the 'Russian-Lego' approach for linear systems, phenomenological models, and specific shortcuts for deriving the key properties of industrial processes. With an emphasis on real-world problems and applications, step-by step modeling design guidelines, and detailed exercises for self-assessment, this is a must-have guide for practitioners and researchers working in chemical, biochemical, food and pharmaceutical engineering.

The book summarises the outcom of a priority research programme: 'Analysis, Modelling and Computation of Multiphase Flows'. The results of 24 individual research projects are presented. The main objective of the research programme was to provide a better understanding of the physical basis for multiphase gas-liquid flows as they are found in numerous chemical and biochemical reactors. The research comprises steady and unsteady multiphase flows in three frequently found reactor configurations, namely bubble columns

without interiors, airlift loop reactors, and aerated stirred vessels. For this purpose new and improved measurement techniques were developed. From the resulting knowledge and data, new and refined models for describing the underlying physical processes were developed, which were used for the establishment and improvement of analytic as well as numerical methods for predicting multiphase reactors. Thereby, the development, lay-out and scale-up of such processes should be possible on a more reliable basis.

This innovative reference provides a coherent and critical view on the potential benefits of a transition from batch to continuous processes in the biopharmaceutical industry, with the main focus on chromatography. It also covers the key topics of protein stability and protein conjugation, addressing the chemical reaction and purification aspects together with their integration. This book offers a fine balance between theoretical modelling and illustrative case studies, between fundamental concepts and applied examples from the academic and industrial literature. Scientists interested in the design of biopharmaceutical processes will find useful practical methodologies, in particular for single-column and multi-column chromatographic processes.

This book outlines a possible future theoretical perspective for systemics, its conceptual morphology and landscape while the Good-Old-Fashioned-Systemics (GOFS) era is still under way. The change from GOFS to future systemics can be represented, as shown in the book title, by the conceptual change from Collective Beings to Quasi-systems. With the current advancements, problems and approaches occurring in contemporary science, systemics are moving beyond the traditional frameworks used in the past. From Collective Beings to Coherent Quasi-Systems outlines a conceptual morphology and landscape for a new

theoretical perspective for systemics introducing the concept of Quasi-systems. Advances in domains such as theoretical physics, philosophy of science, cell biology, neuroscience, experimental economics, network science and many others offer new concepts and technical tools to support the creation of a fully transdisciplinary General Theory of Change. This circumstance requires a deep reformulation of systemics, without forgetting the achievements of established conventions. The book is divided into two parts. Part I, examines classic systemic issues from new theoretical perspectives and approaches. A new general unified framework is introduced to help deal with topics such as dynamic structural coherence and Quasi-systems. This new theoretical framework is compared and contrasted with the traditional approaches. Part II focuses on the process of translation into social culture of the theoretical principles, models and approaches introduced in Part I. This translation is urgent in post-industrial societies where emergent processes and problems are still dealt with by using the classical or non-systemic knowledge of the industrial phase.

Within the last decade, several industrialized countries have stressed the importance of advanced manufacturing to their economies. Many of these plans have highlighted the development of additive manufacturing techniques, such as 3D printing which, as of 2018, are still in their infancy. The objective is to develop superior products, produced at lower overall operational costs. For these goals to be realized, a deep understanding of the essential ingredients comprising the materials involved in additive manufacturing is needed. The combination of rigorous material modeling theories, coupled with the dramatic increase of computational power can potentially play a significant role in the analysis, control, and design of many emerging additive manufacturing processes. Specialized materials and the precise

design of their properties are key factors in the processes. Specifically, particle-functionalized materials play a central role in this field, in three main regimes: (1) to enhance overall filament-based material properties, by embedding particles within a binder, which is then passed through a heating element and the deposited onto a surface, (2) to “functionalize” inks by adding particles to freely flowing solvents forming a mixture, which is then deposited onto a surface and (3) to directly deposit particles, as dry powders, onto surfaces and then to heat them with a laser, e-beam or other external source, in order to fuse them into place. The goal of these processes is primarily to build surface structures which are extremely difficult to construct using classical manufacturing methods. The objective of this monograph is introduce the readers to basic techniques which can allow them to rapidly develop and analyze particulate-based materials needed in such additive manufacturing processes. This monograph is broken into two main parts: “Continuum Method” (CM) approaches and “Discrete Element Method” (DEM) approaches. The materials associated with methods (1) and (2) are closely related types of continua (particles embedded in a continuous binder) and are treated using continuum approaches. The materials in method (3), which are of a discrete particulate character, are analyzed using discrete element methods.

The first comprehensive guide to chemical looping partial oxidation processes, covering key principles, techniques, and applications.

This book is a monography about perfusion cell cultures for the production of biopharmaceuticals, such as therapeutic proteins (i.e. biomolecules like monoclonal antibodies), and describes the fundamentals, design and operation of these processes. Context is given in the first chapters to understand the state-of-the-art of the technology. We

then give an overview of the challenges and objectives in operating mammalian cell perfusion cultures and provide guidelines for the design and setup of lab-scale bioreactor systems, and the required control structure to achieve stable operation. Scale-down devices and PAT tools are described in the context of continuous manufacturing and guidelines for process optimization are given using a variety of case studies to illustrate different approaches. Scale-up is also adressed with a strong focus on bioreactor aeration and mixing, shear stress and cell retention device. Finally, a general introduction for the application of mechanistic and statistic models in bioreactor process development and optimization is given in the last chapter.

This book concerns the most up-to-date advances in computational transport phenomena (CTP), an emerging tool for the design of gas-solid processes such as fluidized bed systems. The authors examine recent work in kinetic theory and CTP and illustrate gas-solid processes' many applications in the energy, chemical, pharmaceutical, and food industries. They also discuss the kinetic theory approach in developing constitutive equations for gas-solid flow systems and how it has advanced over the last decade as well as the possibility of obtaining innovative designs for multiphase reactors, such as those needed to capture CO2 from flue gases. Suitable as a concise reference and a textbook supplement for graduate courses, Computational Transport Phenomena of Gas-Solid Systems is ideal for practitioners in industries involved with the design and operation of processes based on fluid/particle mixtures, such as the energy, chemicals, pharmaceuticals, and food processing.

All-inclusive introduction to polydisperse multiphase flows linking theory to

practice through numerous real-world examples and MATLAB scripts for key algorithms.

Presents the fundamentals of chemical engineering fluid mechanics with an emphasis on valid and practical approximations in modeling.

Advances of Computational Fluid Dynamics in Nuclear Reactor Design and Safety Assessment presents the latest computational fluid dynamic technologies. It includes an evaluation of safety systems for reactors using CFD and their design, the modeling of Severe Accident Phenomena Using CFD, Model Development for Two-phase Flows, and Applications for Sodium and Molten Salt Reactor Designs. Editors Joshi and Nayak have an invaluable wealth of experience that enables them to comment on the development of CFD models, the technologies currently in practice, and the future of CFD in nuclear reactors. Readers will find a thematic discussion on each aspect of CFD applications for the design and safety assessment of Gen II to Gen IV reactor concepts that will help them develop cost reduction strategies for nuclear power plants. Presents a thematic and comprehensive discussion on each aspect of CFD applications for the design and safety assessment of nuclear reactors Provides an historical review of the development of CFD models, discusses state-of-the-art concepts, and takes an applied and analytic look toward the future Includes CFD tools and

simulations to advise and guide the reader through enhancing cost effectiveness, safety and performance optimization

This book describes theories for granular flow based on continuum models and alternative discrete models.

Describes dynamic state of metabolic systems, while paving the way for fully predictive modeling frameworks.

Explore and review novel techniques for intensifying transport and reaction in liquid-liquid and related systems with this essential toolkit. Topics include discussion of the principles of process intensification, the nexus between process intensification and sustainable engineering, and the fundamentals of liquid-liquid contacting, from an expert with over forty-five years' experience in the field. Providing promising directions for investment and for new research in process intensification, in addition to a unique review of the fundamentals of the topic, this book is the perfect guide for senior undergraduate students, graduate students, developers, and research staff in chemical engineering and biochemical engineering.

Building up gradually from first principles, this unique introduction to modern thermodynamics integrates classical, statistical and molecular approaches and is especially designed to support students studying chemical and biochemical

engineering. In addition to covering traditional problems in engineering thermodynamics in the context of biology and materials chemistry, students are also introduced to the thermodynamics of DNA, proteins, polymers and surfaces. It includes over 80 detailed worked examples, covering a broad range of scenarios such as fuel cell efficiency, DNA/protein binding, semiconductor manufacturing and polymer foaming, emphasizing the practical real-world applications of thermodynamic principles; more than 300 carefully tailored homework problems, designed to stretch and extend students' understanding of key topics, accompanied by an online solution manual for instructors; and all the necessary mathematical background, plus resources summarizing commonly used symbols, useful equations of state, microscopic balances for open systems, and links to useful online tools and datasets.

An essential text on practical application, theory and simulation, written by an international coalition of experts in the field and edited by the authors of Colloidal Suspension Rheology. This up-to-date work builds upon the prior work as a valuable guide to formulation and processing, as well as fundamental rheology of colloidal suspensions. Thematically, theory and simulation are connected to industrial application by consideration of colloidal interactions, particle properties, and suspension microstructure. Important classes of model suspensions

including gels, glasses and soft particles are covered so as to develop a deeper understanding of industrial systems ranging from carbon black slurries, paints and coatings, asphalt, cement, and mine tailings, to natural suspensions such as biocolloids, protein solutions, and blood. Systematically presenting the established facts in this multidisciplinary field, this book is the perfect aid for academic researchers, graduate students, and industrial practitioners alike.
This book describes the most widely applicable modeling approaches. Chapters are organized in six groups covering from fundamentals to relevant applications. The book covers particle-based methods and also discusses Eulerian-Eulerian and Eulerian-Lagrangian techniques based on finite-volume schemes. Moreover, the possibility of modeling the poly-dispersity of the secondary phases in Eulerian-Eulerian schemes by solving the population balance equation is discussed.
The era of the fourth industrial revolution has fundamentally transformed the manufacturing landscape. Products are getting increasingly complex and customers expect a higher level of customization and quality. Manufacturing in the Era of 4th Industrial Revolution explores three technologies that are the building blocks of the next-generation advanced manufacturing.The first technology covered in Volume 1 is Additive Manufacturing (AM). AM has emerged as a very popular manufacturing process. The most common form of

AM is referred to as 'three-dimensional (3D) printing'. Overall, the revolution of additive manufacturing has led to many opportunities in fabricating complex, customized, and novel products. As the number of printable materials increases and AM processes evolve, manufacturing capabilities for future engineering systems will expand rapidly, resulting in a completely new paradigm for solving a myriad of global problems.The second technology is industrial robots, which is covered in Volume 2 on Robotics. Traditionally, industrial robots have been used on mass production lines, where the same manufacturing operation is repeated many times. Recent advances in human-safe industrial robots present an opportunity for creating hybrid work cells, where humans and robots can collaborate in close physical proximities. This Cobots, or collaborative robots, has opened up to opportunity for humans and robots to work more closely together. Recent advances in artificial intelligence are striving to make industrial robots more agile, with the ability to adapt to changing environments and tasks. Additionally, recent advances in force and tactile sensing enable robots to be used in complex manufacturing tasks. These new capabilities are expanding the role of robotics in manufacturing operations and leading to significant growth in the industrial robotics area.The third technology covered in Volume 3 is augmented and virtual reality. Augmented and virtual reality (AR/VR)

technologies are being leveraged by the manufacturing community to improve operations in a wide variety of ways. Traditional applications have included operator training and design visualization, with more recent applications including interactive design and manufacturing planning, human and robot interactions, ergonomic analysis, information and knowledge capture, and manufacturing simulation. The advent of low-cost solutions in these areas is accepted to accelerate the rate of adoption of these technologies in the manufacturing and related sectors.Consisting of chapters by leading experts in the world, Manufacturing in the Era of 4th Industrial Revolution provides a reference set for supporting graduate programs in the advanced manufacturing area.

Doctoral Thesis / Dissertation from the year 2013 in the subject Engineering - Mechanical Engineering, grade: 1, University of Linz (Department on Particulate Flow Modelling), language: English, abstract: The numerical hybrid model EUgran+, which is an Eulerian-Eulerian granular phase model extended with models from the Eulerian-Lagrangian model for dense rapid particulate flows, is modified to account for poly-dispersed particle diameter distributions. These modifications include the implementation of I) a new poly-dispersed drag law and of II) new particle boundary conditions distinguishing between sliding and non-sliding particle-wall collisions and III) a new implementation of the population

balance equation in the agglomeration model using the Eulerian-Lagrangian approach, referred to as Bus-stop model. Further, the applicability of the EUgran+ model is extended to cover dilute to dense poly-disperse particulate flows. Furthermore, this provides an improvement in the numerical simulation of dust separation and the formation of particle strands in industrial scale cyclones. In this PHD thesis, the EUgran+Poly model is validated at 3 specific cases with different mass loadings: I) poly-dispersed particle conveying in a square pipe with a 90 degree bend at low mass loading (L = 0:00206); II) a particle conveying case in a rectangular pipe with a double-loop at high mass loading (L = 1:5); III) in a vertical pipe the implementation of the agglomeration model is validated. To show the applicability of the presented models a simulation of an industrial cyclone in experimental scale is presented. The validation and application shows that considering a poly-disperse Eulerian-Eulerian granular phase improves the accordance of the simulation results with measurements significantly. Finally, the hybrid model is a good compromise for a computational efficient simulation of particulate transport and separation with different mass loading regimes.

Providing a clear description of the theory of polydisperse multiphase flows, with emphasis on the mesoscale modelling approach and its relationship with microscale and macroscale models, this all-inclusive introduction is ideal whether

you are working in industry or academia. Theory is linked to practice through discussions of key real-world cases (particle/droplet/bubble coalescence, break-up, nucleation, advection and diffusion and physical- and phase-space), providing valuable experience in simulating systems that can be applied to your own applications. Practical cases of QMOM, DQMOM, CQMOM, EQMOM and ECQMOM are also discussed and compared, as are realizable finite-volume methods. This provides the tools you need to use quadrature-based moment methods, choose from the many available options, and design high-order numerical methods that guarantee realizable moment sets. In addition to the numerous practical examples, MATLAB scripts for several algorithms are also provided, so you can apply the methods described to practical problems straight away.

The go-to guide to learn the principles and practices of design and analysis in chemical engineering.

The Special Issue presents almost 40 papers on recent research in modeling of pyrometallurgical systems, including physical models, first-principles models, detailed CFD and DEM models as well as statistical models or models based on machine learning. The models cover the whole production chain from raw materials processing through the reduction and conversion unit processes to

ladle treatment, casting, and rolling. The papers illustrate how models can be used for shedding light on complex and inaccessible processes characterized by high temperatures and hostile environment, in order to improve process performance, product quality, or yield and to reduce the requirements of virgin raw materials and to suppress harmful emissions.

Computational Models for Polydisperse Particulate and Multiphase SystemsCambridge University Press

Understand common scheduling as well as other advanced operational problems with this valuable reference from a recognized leader in the field. Beginning with basic principles and an overview of linear and mixed-integer programming, this unified treatment introduces the fundamental ideas underpinning most modeling approaches, and will allow you to easily develop your own models. With more than 150 figures, the basic concepts and ideas behind the development of different approaches are clearly illustrated. Addresses a wide range of problems arising in diverse industrial sectors, from oil and gas to fine chemicals, and from commodity chemicals to food manufacturing. A perfect resource for engineering and computer science students, researchers working in the area, and industrial practitioners.

Bridging Scales in Modelling and Simulating Reacting Flows, Part I , Volume 52 presents key

methods to bridge scales in the simulation of reacting single phase flows. New sections in the updated release include topics such as quadrature-based moment methods for multiphase chemically reacting flows, the collaboration of experiments and simulations for the development of predictive models, a simulation of turbulent coalescence and breakage of bubbles and droplets in the presence of surfactants, a section on salts and contaminants, and information on the numerical simulation of reactive flows. Contains reviews by leading authorities in their respective areas Presents up-to-date reviews of the latest techniques in the modeling of catalytic processes Includes a broad mix of US and European authors, as well as academic, industrial and research institute perspectives Provides discussions on the connections between computational and experimental methods

The development of computational methods that support human health and environmental risk assessment of engineered nanomaterials has attracted great interest because the application of these methods enables us to fill existing experimental data gaps. However, considering the high degree of complexity and multifunctionality of engineered nanoparticles, computational methods originally developed for regular (i.e., classic) chemicals cannot always be applied explicitly in nanotoxicology. Thus, the main idea of this book is to discuss the current state of the art and future needs in the development of computational modeling techniques for nanotoxicology. The book focuses on methodology. Among various in silico techniques, special attention is given to (i) computational chemistry (quantum mechanics, semi-empirical methods, density functional theory, molecular mechanics, molecular dynamics); (ii) nanochemoinformatic methods (quantitative structure–activity relationship modeling, grouping, read-across); and (iii) nanobioinformatic methods (genomics, transcriptomics, proteomics,

metabolomics).

A unique text covering basic and advanced concepts of optimization theory and methods for process systems engineers. With examples illustrating key concepts and algorithms, and exercises involving theoretical derivations, numerical problems and modeling systems, it is ideal for single-semester, graduate courses in process systems engineering.

Master the principles of thermodynamics, and understand their practical real-world applications, with this deep and intuitive undergraduate textbook.

This book contains selected papers of the 11th OpenFOAM® Workshop that was held in Guimarães, Portugal, June 26 - 30, 2016. The 11th OpenFOAM® Workshop had more than 140 technical/scientific presentations and 30 courses, and was attended by circa 300 individuals, representing 180 institutions and 30 countries, from all continents. The OpenFOAM® Workshop provided a forum for researchers, industrial users, software developers, consultants and academics working with OpenFOAM® technology. The central part of the Workshop was the two-day conference, where presentations and posters on industrial applications and academic research were shown. OpenFOAM® (Open Source Field Operation and Manipulation) is a free, open source computational toolbox that has a larger user base across most areas of engineering and science, from both commercial and academic organizations. As a technology, OpenFOAM® provides an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics, among several others. Additionally, the OpenFOAM technology offers complete freedom to customize and extend its functionalities.

This book develops the theoretical foundations of disperse two-phase flows, which are

characterized by the existence of bubbles, droplets or solid particles finely dispersed in a carrier fluid, which can be a liquid or a gas. Chapters clarify many difficult subjects, including modeling of the interfacial area concentration. Basic knowledge of the subjects treated in this book is essential to practitioners of Computational Fluid Dynamics for two-phase flows in a variety of industrial and environmental settings. The author provides a complete derivation of the basic equations, followed by more advanced subjects like turbulence equations for the two phases (continuous and disperse) and multi-size particulate flow modeling. As well as theoretical material, readers will discover chapters concerned with closure relations and numerical issues. Many physical models are presented, covering key subjects including heat and mass transfers between phases, interfacial forces and fluid particles coalescence and breakup, amongst others. This book is highly suitable for students in the subject area, but may also be a useful reference text for more advanced scientists and engineers.

Address physical principles and unified theories governing multiphase flows, with methods, applications, and problems.

Learn classical thermodynamics alongside statistical mechanics and how macroscopic and microscopic ideas interweave with this fresh approach to the subjects.

With this unique and comprehensive text, readers will gain the quantitative tools needed to engineer the particulate processes and products that are ubiquitous in modern life. Covering a series of particle and particulate delivery form design processes, with emphasis on design and operation to control particle attributes, and supported by many worked examples, it is essential reading for students and

practitioners. Topics covered include a range of particle design processes such as crystallization and precipitation, granulation, grinding, aerosol processes and spray drying, as well as forms of delivery such as granules, tablets, dry powders, and aerosols. Readers will learn from real-world examples how the primary particle properties and the structure and properties of the delivery form can lead to high performance products, ranging from pharmaceuticals, consumer goods and foods, to specialty chemicals, paints, agricultural chemicals and minerals. Multiphase Particulate Systems in Turbulent Flows: Fluid-Liquid and Solid-Liquid Dispersions provides methods necessary to analyze complex particulate systems and related phenomena including physical, chemical and mathematical description of fundamental processes influencing crystal size and shape, suspension rheology, interfacial area of drops and bubbles in extractors and bubble columns. Examples of mathematical model formulation for different processes taking place in such systems is shown. Discussing connections between turbulent mixing mechanisms and precipitation, it discusses influence of fine-scale structure of turbulence, including its intermittent character, on breakage of drops, bubbles, cells, plant cell aggregates. An important aspect of the mathematical modeling presented in the book is multi-fractal, taking into account the influence of internal intermittency on different phenomena. Key

Features Provides detailed descriptions of dispersion processes in turbulent flow, interactions between dispersed entities, and continuous phase in a single volume Includes simulation models and validation experiments for liquid-liquid, gas-liquid, and solid-liquid dispersions in turbulent flows Helps reader learn formulation of mathematical models of breakage or aggregation processes using multifractal theory Explains how to solve different forms of population balance equations Presents a combination of theoretical and engineering approaches to particulate systems along with discussion of related diversity, with exercises and case studies

"Optimization for Chemical and Biochemical Engineering - Theory, Algorithms, Modeling and Applications"--

Since their first introduction in natural sciences through the work of Einstein on Brownian motion in 1905 and further works, in particular by Langevin, Smoluchowski and others, stochastic processes have been used in several areas of science and technology. For example, they have been applied in chemical studies, or in fluid turbulence and for combustion and reactive flows. The articles in this book provide a general and unified framework in which stochastic processes are presented as modeling tools for various issues in engineering, physics and chemistry, with particular focus on fluid mechanics and notably

dispersed two-phase flows. The aim is to develop what can referred to as stochastic modeling for a whole range of applications.

This study presents the basic models for discrete and continuous particle laden flow simulation. An overview of the two main approaches, the Lagrangian discrete particle model and the Eulerian granular phase model is given. Moreover these two approaches are combined to a hybrid model to use the benefits of the discrete and continuous description. This safes computational time and increase the efficiency of particle laden flow simulations. Furthermore the models are extended to poly-disperse particles including a simple agglomeration model based on a population balance equation. Finally the usability of the models is shown at a pneumatic particle transport system including particle strand building and the separation of particles using an industrial cyclone.

This undergraduate textbook integrates the teaching of numerical methods and programming with problems from core chemical engineering subjects.

A fresh look to process control. State-space and traditional approaches presented in parallel with relevant computer software.