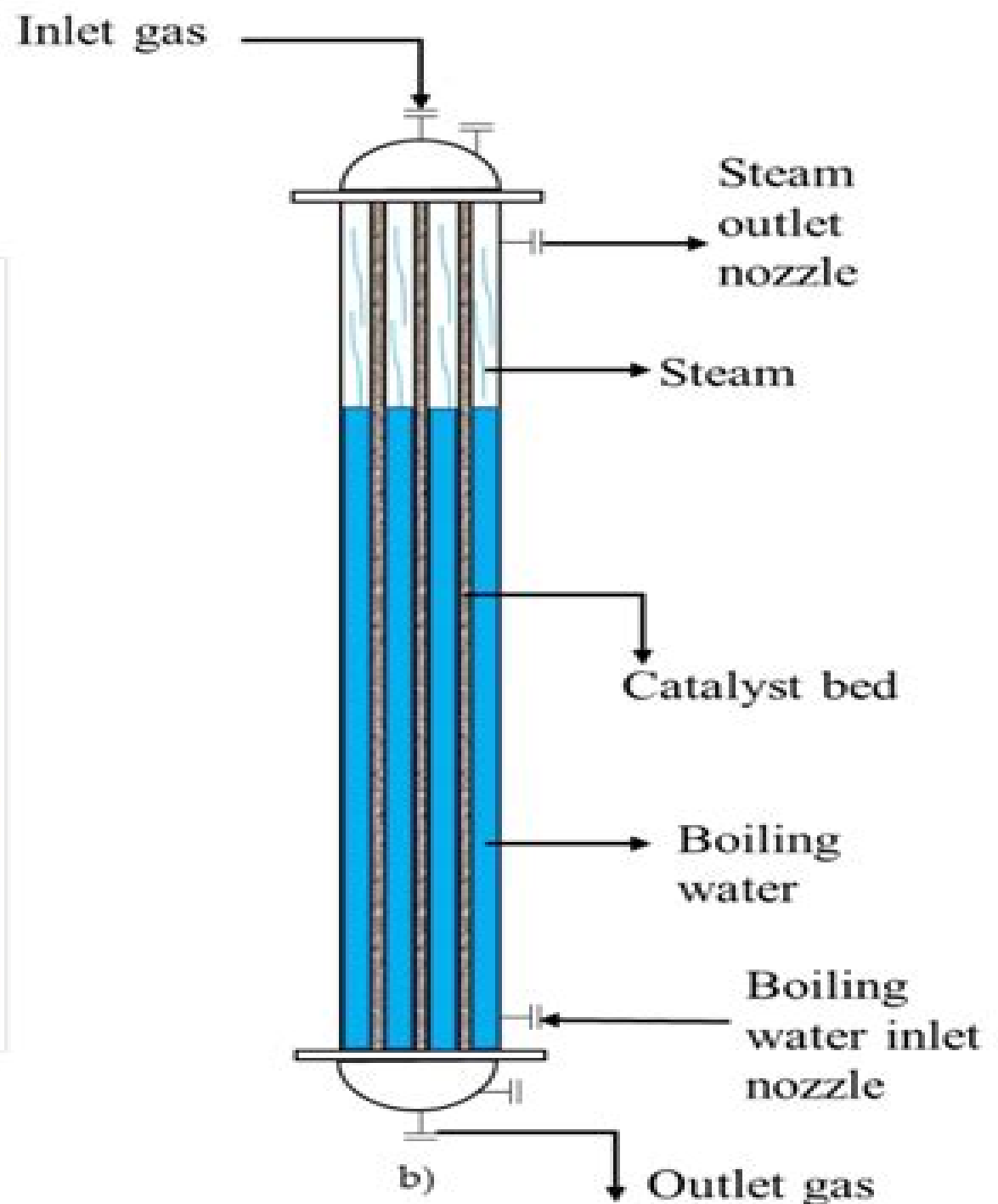




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Mathematical Modeling of Complex Reaction Systems in the Oil and Gas Industry Jorge Ancheyta, Andrey Zagoruiko, Andrey Elyshev, 2024-09-30 Master the fundamentals of reaction systems modeling for the age of decarbonization Reactor design is one of the most important parts of the oil and gas industry with reactor processes and the accompanying technologies constantly evolving to meet industry needs A crucial component of effective reactor design is modelling complex reaction systems which can help predict commercial performance shape safety procedures and more At a time when decarbonization and clean energy transition are among the fundamental global technological challenges it has never been more important for engineers to grasp the cutting edge of reaction system modelling Mathematical Modeling of Complex Reaction Systems in the Oil and Gas Industry provides a systematic introduction to this timely subject Each chapter provides a step by step description of the kinetic and reactor models for a particular kind of process and its accompanying systems Backed by voluminous experimental data and incorporating extensive simulation results the book constitutes an indispensable contribution to the global search for clean energy solutions Mathematical Modeling of Complex Reaction Systems in the Oil and Gas Industry readers will also find All the required tools for developing new reactor models for different reaction scales Detailed discussion of topics including hydrocracking of heavy oils catalyst deactivation oxidative regeneration of catalysts and many more Extensive treatment of both steady state and dynamic simulations Mathematical Modeling of Complex Reaction Systems in the Oil and Gas Industry is ideal for chemical and process engineers computational chemists and modelers catalysis researchers and any other researchers or professionals in petrochemical engineering and the oil and gas industry

Modeling and Simulation of Catalytic Reactors for Petroleum Refining Jorge Ancheyta, 2011-04-20 Modeling and Simulation of Catalytic Reactors for Petroleum Refining deals with fundamental descriptions of the main conversion processes employed in the petroleum refining industry catalytic hydrotreating catalytic reforming and fluid catalytic cracking Common approaches for modeling of catalytic reactors for steady state and dynamic simulations are also described and analyzed Aspects such as thermodynamics reaction kinetics process variables process scheme and reactor design are discussed in detail from both research and commercial points of view Results of simulation with the developed models are compared with those determined at pilot plant scale as well as commercial practice Kinetics data used in the reactor model are either taken from the literature or obtained under controlled experiments at the laboratory

Chemical Reactor Modeling Hugo A. Jakobsen, 2014-04-02 Chemical Reactor Modeling closes the gap between Chemical Reaction Engineering and Fluid Mechanics The second edition consists of two volumes Volume 1 Fundamentals Volume 2 Chemical Engineering Applications In volume 1 most of the fundamental theory is presented A few numerical model simulation application examples are given to elucidate the link between theory and applications In volume 2 the chemical reactor equipment to be modeled are described Several engineering models are introduced and discussed A survey

of the frequently used numerical methods algorithms and schemes is provided A few practical engineering applications of the modeling tools are presented and discussed The working principles of several experimental techniques employed in order to get data for model validation are outlined The monograph is based on lectures regularly taught in the fourth and fifth years graduate courses in transport phenomena and chemical reactor modeling and in a post graduate course in modern reactor modeling at the Norwegian University of Science and Technology Department of Chemical Engineering Trondheim Norway The objective of the book is to present the fundamentals of the single fluid and multi fluid models for the analysis of single and multiphase reactive flows in chemical reactors with a chemical reactor engineering rather than mathematical bias Organized into 13 chapters it combines theoretical aspects and practical applications and covers some of the recent research in several areas of chemical reactor engineering This book contains a survey of the modern literature in the field of chemical reactor modeling

Advances in Synthesis Gas: Methods, Technologies and Applications Mohammad Reza

Rahimpour, Mohammad Amin Makarem, Maryam Meshksar, 2022-10-18 Advances in Synthesis Gas Methods Technologies and Applications Syngas Process Modelling and Apparatus Simulation consists of numerical modeling and simulation of different processes and apparatus for producing syngas purifying it as well as synthesizing different chemical materials or generating heat and energy from syngas These apparatus and processes include but are not limited to reforming gasification partial oxidation swing technologies and membranes Introduces numerical modeling and the simulation of syngas production processes and apparatus Describes numerical models and simulation procedures utilized for syngas purification processes and equipment Discusses modelling and simulation of processes using syngas as a source for producing chemicals and power

Multiscale and Innovative Kinetic Approaches in Heterogeneous Catalysis Pascal Granger, Yves Schuurman, 2019-07-11 Kinetics and reactor modeling for heterogeneous catalytic reactions are prominent tools for investigating and understanding catalyst functionalities at nanoscale and the related rates of complex reaction networks This book illustrates some examples related to the transformation of simple to more complex feedstocks including different types of reactor designs i e steady state transient plug flow reactors and TAP reactors for which there is sometimes a strong gap in the operating conditions from ultra high vacuum to high pressure conditions In conjunction new methodologies have emerged giving rise to more robust microkinetics models As exemplified they include the kinetics and the dynamics of the reactors and span a large range of length and time scales The objective of this Special Issue is to provide contributions that can illustrate recent advances and novel methodologies for elucidating the kinetics of heterogeneous reactions and the necessary multiscale approach for optimizing the reactor design This book is dedicated to postgraduate and scientific researchers and experts in heterogeneous catalysis It may also serve as a source of original information for the elaboration of lessons on catalysis for Master students

Multiphase Catalytic Reactors Zeynep Ilse Önsan, Ahmet Kerim Avci, 2016-06-09 Provides a holistic approach to multiphase catalytic reactors from their modeling and design to their applications in industrial manufacturing of chemicals

Covers theoretical aspects and examples of fixed bed fluidized bed trickle bed slurry monolith and microchannel reactors
Includes chapters covering experimental techniques and practical guidelines for lab scale testing of multiphase reactors
Includes mathematical content focused on design equations and empirical relationships characterizing different multiphase reactor types together with an assortment of computational tools Involves detailed coverage of multiphase reactor applications such as Fischer Tropsch synthesis fuel processing for fuel cells hydrotreating of oil fractions and biofuels processing

12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering, 2015-07-14 25th European Symposium on Computer Aided Process Engineering contains the papers presented at the 12th Process Systems Engineering PSE and 25th European Society of Computer Aided Process Engineering ESCAPE Joint Event held in Copenhagen Denmark 31 May 4 June 2015 The purpose of these series is to bring together the international community of researchers and engineers who are interested in computing based methods in process engineering This conference highlights the contributions of the PSE CAPE community towards the sustainability of modern society Contributors from academia and industry establish the core products of PSE CAPE define the new and changing scope of our results and future challenges Plenary and keynote lectures discuss real world challenges globalization energy environment and health and contribute to discussions on the widening scope of PSE CAPE versus the consolidation of the core topics of PSE CAPE Highlights how the Process Systems Engineering Computer Aided Process Engineering community contributes to the sustainability of modern society Presents findings and discussions from both the 12th Process Systems Engineering PSE and 25th European Society of Computer Aided Process Engineering ESCAPE Events Establishes the core products of Process Systems Engineering Computer Aided Process Engineering Defines the future challenges of the Process Systems Engineering Computer Aided Process Engineering community

Periodic Operation of Chemical Reactors P. L. Silveston, R. R. Hudgins, 2012-12-04 This comprehensive review prepared by 24 experts many of whom are pioneers of the subject brings together in one place over 40 years of research in this unique publication This book will assist R provides a rich source of experimental data plus process models Accompanying website with modelling data

Introduction to Chemical Reactor Analysis R.E. Hayes, J.P. Mmbaga, 2012-10-05 Introduction to Chemical Reactor Analysis Second Edition introduces the basic concepts of chemical reactor analysis and design an important foundation for understanding chemical reactors which play a central role in most industrial chemical plants The scope of the second edition has been significantly enhanced and the content reorganized for im

Chemical Reaction Engineering Tapio Salmi, Johan Wärnå, José Rafael Hernández Carucci, César A. de Araújo Filho, 2023-07-24 Follow step by step explanations to understand mathematical models algebraic and differential equations of chemical reactors and how numerical models work in computer implementation Learn the basics behind current user friendly tools in numerical simulation and optimization of reactor systems Python Matlab Julia and gPROMS Discover how to select the right algorithm for specific reactor models from homogenous to

multiphase systems and structured reactors in detailed discussions at the end of each chapter In this second edition 20 solved example simulations performed in MATLAB and Python are included for demonstration purposes Download solutions to exercises in the book <http://web.abo.fi/fak/tek/cre> **Simulation and Modeling Methodologies, Technologies and Applications** Mohammad S. Obaidat, Tuncer Oren, Floriano De Rango, 2021-08-07 This book includes a set of selected best extended papers from the 10th International Conference on Simulation and Modeling Methodologies Technologies and Applications SIMULTECH 2020 that was held as an online event from July 8 to 10 2020 The conference brought together researchers engineers and practitioners interested in methodologies and applications of modeling and simulation New and innovative solutions are reported in this book A selection was made after the conference based also on the conference chairs assessment reviewers assessment quality of presentation and audience interest so that this book includes the extended and revised versions of the very best papers of the conference **Kinetics and Reactor Design** EduGorilla Prep

Experts, 2024-07-07 EduGorilla Publication is a trusted name in the education sector committed to empowering learners with high quality study materials and resources Specializing in competitive exams and academic support EduGorilla provides comprehensive and well structured content tailored to meet the needs of students across various streams and levels

Advances in Bioenergy Peter D. Lund, John A. Byrne, Goeran Berndes, Iacovos Vasalos, 2015-12-07 The increasing deployment of bioenergy frequently raises issues regarding the use of land and raw materials infrastructure and logistics In light of these sometimes conflicting interests *Advances in Bioenergy* provides an objective and wide ranging overview of the technology economics and policy of bioenergy Offering an authoritative multidisciplinary summary of the opportunities and challenges associated with bioenergy utilization with international researchers give up to date and detailed information on key issues for biomass production and conversion to energy Key features Discusses different bioenergy uses such as transportation fuels electricity and heat production Assesses emerging fields such as bio based chemicals and bio refineries Debates conditions for the mobilization of sustainable bioenergy supply chains and outlines governance systems to support this mobilization Dedicated chapters to sustainability governance and emerging tools such as certification systems and standards supporting growth of a sustainable bioenergy industry Considers the political environmental social and cultural context related to the demand for energy resources the impact of this demand on the world around us and the choices and behaviours of consumers This book will be a vital reference to engineers researchers and students that need an accessible overview of the bioenergy area It will also be of high value for politicians policymakers and industry leaders that need to stay up to date with the state of the art science and technology in this area *Membrane Engineering for the Treatment of Gases: Gas-separation problems combined with membrane reactors* E. Drioli, Giuseppe Barbieri, 2011 This two volume set presents the state of the art and potential for future developments in membrane engineering for the separation of gases

Fuel Cells: Technologies for Fuel Processing Dushyant Shekhawat, J.J. Spivey, David A Berry, 2011-03-18 Fuel Cells

Technologies for Fuel Processing provides an overview of the most important aspects of fuel reforming to the generally interested reader researcher technologist teacher student or engineer The topics covered include all aspects of fuel reforming fundamental chemistry different modes of reforming catalysts catalyst deactivation fuel desulfurization reaction engineering novel reforming concepts thermodynamics heat and mass transfer issues system design and recent research and development While no attempt is made to describe the fuel cell itself there is sufficient description of the fuel cell to show how it affects the fuel reformer By focusing on the fundamentals this book aims to be a source of information now and in the future By avoiding time sensitive information analysis e g economics it serves as a single source of information for scientists and engineers in fuel processing technology The material is presented in such a way that this book will serve as a reference for graduate level courses fuel cell developers and fuel cell researchers Chapters written by experts in each area Extensive bibliography supporting each chapter Detailed index Up to date diagrams and full colour illustrations Synthetic Natural Gas Tilman J. Schildhauer, Serge M. A. Biollaz, 2016-06-15 Provides an overview of the different pathways to produce Synthetic Natural Gas Covers technological and economic aspects of this Synthetic Natural Gas Details the most popular technologies and state of the art of SNG technologies while also covering recent and future research trends Covers the main process steps during conversion of coal and dry biomass to SNG gasification gas cleaning methanation and gas upgrading Describes a number of novel processes for the production of SNG with their specific combination of process steps as well as the boundary conditions Covers important technical aspects of Power to Gas processes Advances in Natural Gas: Formation, Processing, and Applications. Volume 8: Natural Gas Process Modelling and Simulation Mohammad Reza Rahimpour, Mohammad Amin Makarem, Maryam Meshksar, 2024-05-11 Advances in Natural Gas Formation Processing and Applications is a comprehensive eight volume set of books that discusses in detail the theoretical basics and practical methods of various aspects of natural gas from exploration and extraction to synthesizing processing and purifying producing valuable chemicals and energy The volumes introduce transportation and storage challenges as well as hydrates formation extraction and prevention Volume 8 titled Process Modelling and Simulation discusses various aspects of natural gas related processes from modelling and simulation point of view This includes modelling of natural gas sweetening dehydration and other impurities removal processes and apparatus as well as simulation of processes and apparatus dealt with producing chemicals and energy from natural gas The book introduces modelling and simulation of natural gas hydrate related processes and covers modelling basics numerical approaches and optimization techniques which provides a deeper understanding of the subject Introduces modelling and simulation methods for natural gas sweetening and purification Describes modelling and simulation procedures of producing chemicals and energy from natural gas Discusses theoretical basics and models of natural gas hydrates *11th International Symposium on Process Systems Engineering - PSE2012*, 2012-12-31 While the PSE community continues its focus on understanding synthesizing modeling designing simulating

analyzing diagnosing operating controlling managing and optimizing a host of chemical and related industries using the systems approach the boundaries of PSE research have expanded considerably over the years While early PSE research was largely concerned with individual units and plants the current research spans wide ranges of scales in size molecules to processing units to plants to global multinational enterprises to global supply chain networks biological cells to ecological webs and time instantaneous molecular interactions to months of plant operation to years of strategic planning The changes and challenges brought about by increasing globalization and the the common global issues of energy sustainability and environment provide the motivation for the theme of PSE2012 Process Systems Engineering and Decision Support for the Flat World Each theme includes an invited chapter based on the plenary presentation by an eminent academic or industrial researcher Reports on the state of the art advances in the various fields of process systems engineering Addresses common global problems and the research being done to solve them

Biowaste and Biomass in Biofuel Applications Yashvir Singh, Vladimir Strezov, Prateek Negi, 2023-02-27 This book reflects the new dimension of biofuel production from its introductory principles to the advancements from a future prospective It summarizes the rationale for changes in liquid fuel utilization and the selection of new technologies to make biofuel cost effective and move toward a carbon neutral approach It provides an evidence based outline of how additives and nanotechnology chemically change biofuels quality and effectiveness including new and innovative approaches such as nanomaterials and various nano additives Features It provides an overview of biowaste as a sustainable source in the field of biofuel production It includes effective conversion parameters of the biowaste feedstocks and their classification It summarizes current research into the development and exploitation of new biofuel sources It discusses the improvement of pilot scale scalability chemical processing and design flow It presents relevant and realistic global explanations of biowaste management techniques for biofuels This book is aimed at senior undergraduate and graduate students and researchers in bioprocessing chemical engineering and biotechnology

Advanced Modelling and Simulation in the Chemical and Biochemical Process Industry Sudip Chakraborty, Stefano Curcio, 2024-10-30 Advanced Modelling and Simulation in the Chemical and Biochemical Process Industry explores modelling and simulation of chemical and biochemical processes at the industrial scale using a variety of approaches Particular attention is devoted to simulations in different scales which help achieve a wide spectrum and more efficient analysis of several problems ranging from the design of novel materials to the optimization of industrial processes as a function of the operating conditions This book not only covers optimization with experimental data but also offers readers a thorough understanding and analysis of different parameters of a whole process stream Covers a wide range of advanced modelling and simulation of chemical technologies ab initio atomistic molecular dynamics MD Lattice Boltzmann LB dissipative particle dynamics DPD computational fluid dynamics CFD and finite element FEM Addresses issues associated with process control in different phases of the chemical industry Features modelling approaches that allow the design of

novel processes materials in a faster and more reliable way This book will be of interest to researchers and advanced readers in chemical biochemical environmental and materials engineering and industrial chemistry

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