Modeling Of Catalyst Fixed Bed Reactor For Production Of

Selecting the best type of reactor for any particular chemical reaction, taking into consideration safety, hazard analysis, scale-up, and many other factors is essential to any industrial problem. An understanding of chemical reaction

kinetics and the design of chemical reactors is key to the success of the of the chemist and the chemical engineer in such an endeavor. This valuable reference volume conveys a basic understanding of chemical reactor design methodologies,

incorporating control, hazard analysis, and other topics not covered in similar texts. In addition to covering fluid mixing, the treatment of wastewater, and chemical reactor modeling, the author includes sections on safety

in chemical reaction and scale-up, two topics that are often neglected or overlooked. As a real-world introduction to the modeling of chemical kinetics and reactor design, the author includes a case study on ammonia synthesis that is

integrated throughout the text. The text also features an accompanying CD, which contains computer programs developed to solve modeling problems using numerical methods. Students, chemists, technologists, and chemical

engineers will all benefit from this comprehensive volume. Shows readers how to select the best reactor design, hazard analysis, and safety in design methodology Features computer programs developed to solve modeling

problems using numerical methods New process technology strategies are required to cope with the future. Fossil feedstocks are losing ground in favour of renewable feedstocks and secondary resources. Conventional processing routes

using thermal `sledgehammer' techniques are replaced by highly selective (bio)catalytic conversions. The future process engineer is neither allowed to think in terms of unit operations, nor to take for granted the conventional practice of

continuous steady state processing. Hybrid systems and transient operations are more and more frequently encountered. The continuing impressive progress being made in process modelling and control will revolutionize the

process industries. In the new generation of chemical production processes the keyword is precision. Precision in terms of selectivity and of efficiency, is required to maximize the utilisation of materials and energy. Moreover, enhanced

precision is needed to exploit the quality of materials and energy to the full extent. Only by reducing the squandering of materials, energy and quality will a harmonious relationship be established between the process industries, the

economy, and the environment. Process integration, as well as an integrated effort by the disciplines involved in process technology, will be of crucial importance in attaining the goals of precision process technology. These emerging

strategies involve an active exchange of tools and ideas between a variety of disciplines, not only in plant design and operation, but even more in the early stages of process development and design. By looking from various angles at

what the future has in store for the process industries, this volume systematically lifts the corners of the veil and may inspire to establish a new tradition of precision in process technology.

The continuous increase in the

global demand for a cleaner energy source has instigated much interest in converting natural gas to ultra-clean fuels and value-added chemicals. Fischer-Tropsch synthesis (FTS) is a key technology for converting syngas, produced

from coal, biomass or natural gas, into a variety of hydrocarbon products. Although this technology has been around for decades, commercial development remains relatively slow and limited to use of few reactor configurations (e.g.

fixed-bed reactor and slurry-bubble column reactor). On the lab-scale, supercritical solvents were utilized in FTS as a reaction media since they have the advantages of both the gas-phase reaction (fixed-bed reactor) and the liquid-phase

reaction (slurry-bubble column reactor), while simultaneously overcoming their limitations. This work focuses on modeling the behavior in the reactor bed ('macro-scale' assessment) and then zooming into the catalyst pellet

itself ('micro-scale' assessment). The aim of this research is to simulate the heat and mass transfer behavior inside the reactor bed, identify typical conditions that look at the existence and absence of both mass and heat transfer

limitations, and to quantify the role of the main controlling parameters on the overall behavior of the reactor bed and on the catalyst effectiveness factor. An often used mathematical model of the fixed-bed reactor was applied to simulate

the concentration and temperature profile simultaneously based on the appropriate mass and heat balances at both scales. A second-order ordinary differential equation was used for a spherical pellet in the radial coordinate for both mass

and heat balances, while a one-dimensional steady state pseudo heterogeneous model was used for the reactor bed modeling in the axial direction. In addition, in both models the mass balance equation was expressed in terms of fugacity

to account for the non-ideal behavior of the reaction mixture in the SCF-FTS. The thermodynamic properties of the mixture were estimated using the Soave-Redlich-Kwong equation of state (SRK-EOS). The simulation results of this

study showed a high temperature rise in the gas-phase FTS relative to that in the SCF-FTS under a comparable reaction conditions. Carbon monoxide conversion was considerably higher in the SCF compared to the gas-phase

reaction. The effect of the particle size on the overall catalyst effectiveness factor was also investigated in both reaction media. The electronic version of this dissertation is accessible from http://hdl.handle.net/1969.1/151762

Modelling and Identification of a Catalytic Packed Bed Reactor
Chemical and Catalytic Reactor Modeling
Optimal Distribution of Catalyst in Pellets, Reactors, and Membranes
Heat And Mass Transfer In Fixed

And Fluidized Beds

Trickle Bed Reactors

Reaction Kinetics and the Development and Operation of Catalytic Processes is a trendsetter. The Keynote Lectures have been authored

by top scientists and cover a broad range of topics like fundamental aspects of surface chemistry, in particular dynamics and spillover, the modeling of reaction mechanisms, with

special focus on the importance of transient experimentation and the application of kinetics in reactor design. Fundamental and applied kinetic studies are well represented. More than

half of these deal with transient kinetics, a new trend made possible by recent sophisticated experimental equipment and the awareness that transient experimentation provides more information and

insight into the microphenomena occurring on the catalyst surface than steady state techniques. The trend is not limited to purely kinetic studies since the great majority of the papers dealing

with reactors also focus on transients and even deliberate transient operation. It is to be expected that this trend will continue and amplify as the community becomes more aware of the predictive

potential of fundamental kinetics when combined with detailed realistic modeling of the reactor operation. Practical Guides in Chemical Engineering are a cluster of short texts that each provides

a focused introductory view on a single subject. The full library spans the main topics in the chemical process industries that engineering professionals require a basic understanding of. They are

'pocket publications' that professional engineers can easily carry with them or access electronically while working. Each text is highly practical and applied, and presents first principles for

engineers who need to get up to speed in a new area fast. The focused facts provided in each guide will help you converse with experts in the field, attempt your own initial troubleshooting, check

calculations, and solve rudimentary problems. Adiabatic Fixed-bed Reactors covers the fundamentals of fixed-bed reactors, including various types and their physical properties.

Applications of each device type are discussed, as well as trouble-shooting Solid-supported Catalysts. This text is ideal for any engineer who is new to working with fixed-bed reactors and needs to

know the basics quickly and easily. Practical, short, concise information on the basics will help you get an answer or teach yourself a new topic quickly Supported by industry examples to help

you solve a real world problem Single subject volumes provide key facts for professionals

The worldwide petroleum industry is facing a dilemma: the production level of heavy

petroleum is higher than that of light petroleum. Heavy crude oils possess high amounts of impurities (sulfur, nitrogen, metals, and asphaltenes), as well as a high yield of residue with

consequent low production of valuable distillates (gasoline and diesel). These characteristics, in turn, are responsible for the low price of heavy petroleum. Additionally, existing

refineries are designed to process light crude oil, and heavy oil cannot be refined to 100 percent. One solution to this problem is the installation of plants for heavy oil upgrading before sending this

raw material to a refinery. Modeling of Processes and Reactors for Upgrading of Heavy Petroleum gives an up-to-date treatment of modeling of reactors employed in the main processes for heavy

petroleum upgrading. The book includes fundamental aspects such as thermodynamics, reaction kinetics, chemistry, and process variables. Process schemes for each process are

discussed in detail. The author thoroughly describes the development of correlations, reactor models, and kinetic models with the aid of experimental data collected from different reaction scales.

The validation of modeling results is performed by comparison with experimental and commercial data taken from the literature or generated in various laboratory scale reactors.

Organized into three sections, this book deals with general aspects of properties and upgrading of heavy oils, describes the modeling of non-catalytic processes, as well as the modeling of catalytic

processes. Each chapter provides detailed experimental data, explanations of how to determine model parameters, and comparisons with reactor model predictions for different situations, so that readers can

adapt their own computer programs. The book includes rigorous treatment of the different topics as well as the step-by-step description of model formulation and application. It is not only an

indispensable reference for professionals working in the development of reactor models for the petroleum industry, but also a textbook for full courses in chemical reaction engineering. The

author would like to express his sincere appreciation to the Marcos Moshinsky Foundation for the financial support provided by means of a Cátedra de Investigación. Modeling and Simulation of

Catalytic Reactors for Petroleum Refining

Catalyst Design

The Modelling and Dynamics of Catalysts and Fixed Bed Reactors

Overview of the New

Developments of Energy and Petrochemical Reactor Technologies. Projections for the 90's

A Three Dimensional Dynamic CFD Simulation for the Direct DME Production in a Fixed

Bed Reactor

Mathematical modelling of gas-solid catalytic reactors in industry is still limited. By consolidating progress in the understanding of

catalytic processes, this book applies fundamental advances to the development of models for design, simulation and optimization of industrial reactors.

In the last two decades impressive advances have been made toward the understanding and quantitative description of the kinetics. Despite these advances, however,

the use of mathematical modelling of gas-solid catalytic reactors in industry is still limited. By consolidating progress in the understanding of catalytic processes, this

book applies these fundamental advances to the development of models for design, simulation and optimization of industrial reactors. Paying particular attention to

the verification of the developed models against industrial data, these models are used to optimize the performance of many practical reactor cases. Using a systems

approach for the development of the different components and the resulting overall models, the book is easy to read and gives an insight into the behaviour

of these complex industrial systems. In addition, the practical relevance of bifurcation, instability and chaos to industrial reactors is briefly discussed.

With petroleum prices spiraling upward, making synthetic fuels-or "synfuels"-from coal, natural gas, and biomass has become more economically competitive.

Advanced energy companies now focus exclusively on alternative fuels, and many oil companies have programs dedicated to developing synthetic fuels. The Fischer-Tropsch

process, which uses a colle

Modelling and Control of a Packed Bed Reactor

Reaction Kinetics and the Development and Operation of Catalytic Processes

CFD Simulation and Experiment of Catalyst Deactivation and Heat Transfer in a Low N Fixed-bed Reactor

Multiphase Catalytic Reactors

Chemical Reactor Omnibook-soft cover

Dimethyl ether (DME) as a clean fuel seems to be a superior candidate for high-quality diesel fuel in near future. In this study, a comprehensive three-

dimensional dynamic heterogeneous model developed to simulate the flow behavior and catalytic coupling reactions for synthesis of the DME from hydrogenation of the CO and CO2, dehydration of methanol

to dimethyl ether and water gas shift reaction in a fixed bed reactor. For this purpose, a CFD simulation was articulated where the standard k-ε model with 10% turbulence tolerations implemented. Then the

concentration and temperature profiles along the reactor were determined. It was revealed that under conditions considered, a single phase physiochemical system under equilibrium existed for which

simulations were performed. Ultimately, generated results of the model under appropriate industrial boundary conditions compared with those of others available in the open literature to verify the

developed model. Then, the effects of various operating parameters including the pressure, temperature and flow rate of the feed to the reactor upon the DME production as well as; selectivity were examined.

The CFD modeling results generated from the present work revealed reasonable agreement with obtained data of these authors and other experimental available in the open literature which considering the complexity

of the task performed was rather satisfying.

Today's frustrations and anxieties resulting from two energy crises in only one decade, show us the problems and fragility of a world built on high energy

consumption, accustomed to the use of cheap non-renewable energy and to the acceptance of eXisting imbalances between the resources and demands of countries. Despite all these stressing factors, our world

is still hesitatins about the urgency of undertaking new and decisive research that could stabilize our future, Could this trend change in the near future? In our view, two different scenarios are possible. A

renewed energy tension could take place with an unpredictable timing mostly related to political and economic factors, This could bring again scientists and technologists to a new state of shock and awaken our

talents, A second interesting and beneficial scenario could result from the positive influence of a new generation of researchers that with or without immediate crisis, acting both in industry and

academia, will face the challenge of developing technologies and processes to pave the way to a less vulnerable society, Because Chemical Reactor Design and Technology activities are at the heart of these required

new technologies the timeliness of the NATO-Advanced Study Institute at the University of Western Ontario, London, was very appropriate.

This work focuses on the development of a computer-

aided modeling framework. The framework is a knowledge-based system that is built on a generic modeling language and structured on workflows for different modeling tasks. The overall objective of this work is to

support model developers and users to generate and test models systematically, efficiently and reliably. In this way, development of products and processes can be made faster, cheaper and more efficient. In this

contribution, as part of the framework a generic modeling template for the systematic derivation of problem specific catalytic membrane fixed bed reactor models is presented. The application of the modeling template is

highlighted with a case study related to the modeling of a catalytic membrane reactor coupling dehydrogenation of ethylbenzene with hydrogenation of nitrobenzene.

Simulation of Fischer-Tropsch Fixed-Bed Reactor in Different Reaction Media

Two phase, two dimensional models of fixed bed catalytic reacto...

Perspectives for Pollution Prevention

Modeling and Simulation of Heterogeneous Catalytic Processes

Parametric Sensitivity in Chemical Systems

Activation, Deactivation, and Poisoning of Catalysts deals with

the circumstances and mechanisms underlying catalyst activation, deactivation, and poisoning. The emphasis is on the techniques for handling deactivating systems, not on results per se. Deactivation by

fouling and sintering is given consideration. This book is organized into three sections and consists of 12 chapters. The first part is devoted to a systematic development of the manner in which catalysts are activated,

deactivated, poisoned, and in some cases reactivated on a microscopic basis. The first chapter explains the concept of the active center as utilized in catalysis, along with catalyst regeneration, rejuvenation, and detoxification.

In the second part, the reader is introduced to the problem of heat transfer as well as the transport of reactants and products in the interior of the particle coupled with chemical reaction therein. The macroscopic deactivation

behavior of the catalyst particle is described in terms of fundamental kinetic deactivation phenomena and of parameters governing heat and mass transfer. The last part is primarily concerned with a collection of catalyst particles

within the reactor, with emphasis on the global activity of the reactor. In the last chapter, a pragmatic approach is presented to predict the design and performance of chemical reactors containing a deactivating catalyst.

This book is written for catalytic chemists, researchers, reactor designers, and students interested in catalyst activation, deactivation, and poisoning. Since heterogeneous catalysis is widely used in chemical, refinery,

and pollution-control processes, achieving optimal catalytic performance is a significant issue for chemical engineers and chemists. This book addresses the question of how catalytic material should be distributed inside a

porous support to obtain optimal performance. It treats single and multiple reaction systems, isothermal and nonisothermal conditions, pellets, monoliths, fixed-bed reactors, and membrane reactors. The effects of

physicochemical and operating parameters are analyzed to gain insight into the underlying phenomena governing the performance of optimally designed catalysts. Throughout, the authors offer a balanced

treatment of theory and experiment and stress problems of commercial importance. 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.

Practical Guides in Chemical Engineering

Modeling of Processes and Reactors for Upgrading of Heavy Petroleum

Catalytic Reactors

Novel Iron Catalyst and Fixed-bed Reactor Model for the Fischer-Tropsch Synthesis

The Method of Volume Averaging

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
Inspired by the leading authority in the field, the Centre for Process Systems Engineering at Imperial College London, this

book includes theoretical developments, algorithms, methodologies and tools in process systems engineering and applications from the chemical, energy, molecular, biomedical and other areas. It

spans a whole range of length scales seen in manufacturing industries, from molecular and nanoscale phenomena to enterprise-wide optimization and control. As such, this will appeal to a broad readership, since the

topic applies not only to all technical processes but also due to the interdisciplinary expertise required to solve the challenge. The ultimate reference work for years to come.

Fluidization Engineering, Second

Edition, expands on its original scope to encompass these new areas and introduces reactor models specifically for these contacting regimes. Completely revised and updated, it is essentially a new book. Its aim is

to distill from the thousands of studies those particular developments that are pertinent for the engineer concerned with predictive methods, for the designer, and for the user and potential user of fluidized beds.

Covers the recent advances in the field of fluidization. Presents the studies of developments necessary to the engineers, designers, and users of fluidized beds.

Activation, Deactivation, and

Poisoning of Catalysts

Nonlinear Analysis in Chemical Engineering
Multiphase Reactive Flows
Fischer-Tropsch Synthesis, Catalysts, and Catalysis

This book provides a hybrid methodology for engineering of trickle bed reactors by integrating conventional reaction engineering models with state-of-the-art

computational flow models. The content may be used in several ways and at various stages in the engineering process: it may be used as a basic resource for making

appropriate reactor engineering decisions in practice; as study material for a course on reactor design, operation, or optimization of trickle bed reactors; or in

solving practical reactor engineering problems. The authors assume some background knowledge of reactor engineering and numerical techniques. Facilitates development of

high fidelity models for industrial applications Facilitates selection and application of appropriate models Guides development and application of computational models to

trickle beds

Multiphase systems dominate nearly every area of science and technology, and the method of volume averaging provides a rigorous foundation for

the analysis of these systems. The development is based on classical continuum physics, and it provides both the spatially smoothed equations and a method of

predicting the effective transport coefficients that appear in those equations. The text is based on a ten-week graduate course that has been taught for more than

20 years at the University of California at Davis and at other universities around the world. Problems dealing with both the theoretical foundations and the applications are

included with each chapter, and detailed solutions for all problems are available from the author. The course has attracted participants from chemical engineering,

mechanical engineering, civil engineering, hydrologic science, mathematics, chemistry and physics.

The Omnibook aims to present the main ideas of

reactor design in a simple and direct way. it includes key formulas, brief explanations, practice exercises, problems from experience and it skims over the

field touching on all sorts of reaction systems. Most important of all it tries to show the reader how to approach the problems of reactor design and what questions to ask.

In effect it tries to show that a common strategy threads its way through all reactor problems, a strategy which involves three factors: identifying the flow patter, knowing

the kinetics, and developing the proper performance equation. It is this common strategy which is the heart of Chemical Reaction Engineering and identifies

it as a distinct field of study.

Chemical Reactor Design and Technology

Theory, Design, Manufacturing, and Applications

Fluidization Engineering

The Simulation of a Fixed Bed Catalytic Reactor, in the Presence of a Rapidly Decaying Catalyst

Catalyst Particle Modelling in Fixed-bed

Reactors

Abstract: Modeling of fluid flow, heat transfer and reaction in fixed beds is an essential part of their design. This is especially critical for highly endothermic reactions

in low tube-to-particle diameter ratio (N) tubes, such as methane steam reforming (MSR) and alkane dehydrogenation as two important commercial reactions. The modeling of

fixed bed reaction is available in literatures with lots of assumptions. However, there is a need for implementing the reaction conditions with diffusion aspects on a real fixed bed reactor without

assuming any pseudo conditions. Computational fluid dynamics (CFD) has been found as a suitable tool by many researchers to simulate fixed beds. CFD can simulate complex geometry of randomly-

packed tubes, and provides us with more fundamental understanding of the transport and reaction phenomena in reactor tubes. CFD can be used to obtain detailed three-dimensional velocity, species

and temperature fields that are needed to improve engineering approaches. Previously, the geometry of 120-degree wall segment (WS) of the whole reactor tube has been studied in our group. Previous works

have introduced the coupling of gas flow and resolved species and temperature gradients inside pellets by CFD for methane steam reforming (MSR) and propane dehydrogenation (PDH)

without considering deactivation. The deactivation of catalysts due to carbon formation is an important problem in industry, such as steam reforming and the catalytic dehydrogenation of

alkanes, which are both strongly endothermic reactions. Many researches were carried out to study the effect of carbon formation and catalyst deactivation on the reactor performance. The local

carbon deposition on catalysts can cause particle breakage and strongly decrease reaction rates. Catalyst deactivation in heated tubes removes the heat sink and can result in local hot spots that weaken the reactor

tube. This is particularly a problem for a low tube-to-particle diameter ratio fixed bed reactor. A 3D resolved CFD model simulation was used to study the local details of carbon deposition in which the

reactions and deactivation take place inside the catalytic solid particles. CFD simulations of flow, heat transfer, diffusion and reaction were carried out using the commercial CFD code FLUENT/ANSYS 6.3 in a

3D 120-degree periodic wall segment with N=4. The mesh used boundary layer prism cells at both the inside and outside particle surfaces and at the tube wall. These reactions were represented in

the solid particles using user-defined scalars to mimic species transport and reaction, with user-defined functions supplying reaction rates. Diffusion in the particles was modeled by Fick's law using an

effective diffusivity, given by Hite and Jackson's approximation of the Dusty Gas Model. The transient developments of particle internal gradients and carbon accumulation have been

studied for the early stages of deactivation. Carbon concentration is initially strongest close to the surface and in the high temperature regions of the catalysts and affected by the wall heat flux.

Deactivation of the endothermic reactions causes a slow increase in the average catalyst temperature. The second stage of the research was the verification of our CFD reaction model with

experimental data under reacting conditions. The highly endothermic commercial methane steam reforming (MSR) reaction was studied experimentally in a fixed bed reactor. The temperature

contributions inside catalyst particles were measured. The MSR reaction showed strong effects on the temperature profile along the reactor. Then, a CFD model was used to predict temperature profiles

under MSR reaction conditions. Comparison of CFD and experimental data showed very good qualitative as well as quantitative agreement for temperature inside catalyst particles at different inlet gas

temperatures. The last stage was to develop a fundamental energy equation without introducing new adjustable parameters to study heat transfer in fixed beds. In the past, many researchers have

been carried out to simulate the heat transfer in fixed bed reactors by using k[subscript r] (effective thermal conductivity) and h[subscript w] (heat transfer coefficient). But the classical model with

k[subscript r] and h[subscript w] cannot give a correct T(r) near tube wall, where deactivation is strongest. Therefore we need a better model which can represent the near wall heat transfer more

accurate. CFD modeling was used to develop pseudo-continuum model for T(r) using V[subscript r] (r, z) and V[subscript z] (r). To get better temperature at the wall vicinity close to the physical

reality. In this model radial thermal conductivity was obtained from Zehner-Schlünder model. The convection heat transfer was calculated in the 2D flow fluid from the CFD run. Results

were obtained for Reynolds numbers in the range 240-?1900. The accuracy of the new model has been validated by analytical solution. The temperature calculated by the new velocity field

pseudohomogenous energy equation showed reasonable quantitative agreement with values predicted by the CFD model.

Modelling, Simulation and Optimization of Industrial

Fixed Bed Catalytic ReactorsCRC Press

Heterogeneous catalysis and mathematical modeling are essential components of the continuing search for better utilization of raw materials and

energy, with reduced impact on the environment. Numerical modeling of chemical systems has progressed rapidly due to increases in computer power, and is used extensively for analysis, design and

development of catalytic reactors and processes. This book presents reviews of the state-of-the-art in modeling of heterogeneous catalytic reactors and processes. Reviews by leading authorities

in the respective areas Up-to-date reviews of latest techniques in modeling of catalytic processes Mix of US and European authors, as well as academic/industrial/research

institute perspectives
Connections between computation and experimental methods in some of the chapters
Adiabatic Fixed-Bed Reactors
Reactor Engineering and

Applications
Modelling, Simulation and Optimization of Industrial Fixed Bed Catalytic Reactors
Catalyst Deactivation and
Fixed Bed Reactor Modeling
Precision Process Technology

This dissertation describes in detail the TFBRRM, reports its validation, and presents results of varying fundamental, theoretically-based parameters (e.g. effective diffusivity, Prandtl number, friction factor, etc.) as well as physical process parameters (i.e. recycle ratio, pressure, flow rate, tube diameter, cooling temperature, and pellet

diameter and shape). For example, the model predicts that decreasing effective diffusivity from 7.1E-9 to 2.8E-9 m^2/s results in a lower maximum temperature (from 523 to 518 K) and a longer required bed length to achieve 60% conversion of CO (from 5.7 to 8.5 m). Using the Tallmadge equation to estimate friction

losses as recommended by the author results in a pressure drop 40% smaller than using the Ergun equation. Validation of the model was accomplished by matching published full-scale plant data from the SASOL Arge reactors.

Catalytic Reactors presents several key aspects of reactor design in Chemical and

Process Engineering. Starting with the fundamental science across a broad interdisciplinary field, this graduate level textbook offers a concise overview on reactor and process design for students, scientists and practitioners new to the field. This book aims to collate into a comprehensive and well-informed work of

leading researchers from north America, western Europe and south-east Asia. The editor and international experts discuss state-of-the-art applications of multifunctional reactors, biocatalytic membrane reactors, micro-flow reactors, industrial catalytic reactors, micro trickle bed reactors and multiphase catalytic reactors. The use of

catalytic reactor technology is essential for the economic viability of the chemical manufacturing industry. The importance of Chemical and Process Engineering and efficient design of reactors are another focus of the book. Especially the combination of advantages from both catalysis and chemical reaction technology for optimization and

intensification as essential factors in the future development of reactors and processes are discussed. Furthermore, options that can drastically influence reaction processes, e.g. choice of catalysts, alternative reaction pathways, mass and heat transfer effects, flow regimes and inherent design of catalytic reactors are reviewed in

detail. Focuses on the state-of-the-art applications of catalytic reactors and optimization in the design and operation of industrial catalytic reactors Insights into transfer of knowledge from laboratory science to industry For students and researchers in Chemical and Mechanical Engineering, Chemistry, Industrial Catalysis

and practising Engineers

The behavior of a chemical system is affected by many physicochemical parameters. The sensitivity of the system's behavior to changes in parameters is known as parametric sensitivity. When a system operates in a parametrically sensitive region, its performance becomes unreliable and

changes sharply with small variations in parameters. Thus, it is of great value to those who design and operate chemical systems to be able to analyze and predict their sensitivity behavior. This book is the first to provide a thorough treatment of the concept of parametric sensitivity and the mathematical tool it generated, sensitivity

analysis. The emphasis is on applications to real situations. The book begins with definitions of various sensitivity indices and describes the numerical techniques most commonly used for their evaluation. Extensively illustrated chapters discuss sensitivity analysis in a variety of chemical reactors--batch, tubular, continuous-flow,

fixed-bed--and in combustion systems, mechanistic studies, air pollution, and metabolic processes. Seniors and graduate students in various fields of science and engineering, researchers, and practicing engineers will welcome this valuable resource.

Computer-aided modeling framework – a

generic modeling template for catalytic membrane fixed bed reactors
Chemical Reaction Engineering
Dynamic Process Modeling
Chemical Reactor Modeling
Advances and Applications

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.

Modeling of Chemical Kinetics and Reactor Design

Modeling of Catalyst Activity and Simulation of a Hybrid Model for a Catalytic Fixed Bed Reactor
Chemical Reactors
23 European Symposium on Computer Aided Process

Engineering