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Chapter 1 : Unsteady catalytic processes and sorption-catalytic technologies - IOPscience

This chapter discusses the catalytic processes in forced unsteady-state conditions. Unsteady-state conditions offer far greater possibilities for forming fields of concentrations, temperatures, and of particular importance, catalyst states that permit one to secure more favorable conditions for the process than those in the steady state.

A potential storage technology is the conversion of electrical energy into chemical energy e. CO2 is the C-source of choice, from biogas plants or industrial processes, making possible the production and use of C-based fuels without increasing the CO2 emissions into the atmosphere. The combination of Fischerâ€"Tropsch synthesis and CO2 shift reaction, using iron-based catalyst, offers the possibility to produce substitute natural gas SNG components from CO2. Due to the fluctuating nature of hydrogen production from renewable electrical energy, advantages can be identified if the chemical reactor is operated under variable load conditions. The aim of the present study is to evaluate the flexibility of a catalytic synthesis reactor as a potential component in a future energy system with a high contribution of renewable energy. The hydrogenation of CO2 to gaseous components is studied in a fixed-bed lab-scale reactor to determine kinetic parameters and hydrocarbon product distribution. Results from the experimental work are implemented in the mathematical model and are the basis for the conceptual design of the catalytic fixed-bed reactor able to operate under variable load conditions. Brunner C, Teufel F. Flexibility in energy systems with a high share of fluctuating renewable energy sources. Balancing renewable electricity â€" energy storage, demand size management, and network extension. Integration erneuerbaren Stroms in das Erdgasnetz, Considerations concerning the energy demand and energy mix for global welfare and stable ecosystems. Chem Ing Tech ; Methanol from atmospheric carbon dioxide: Energy Convers Manage ; Energy and material balance of CO2 capture from ambient air. Environ Sci Technol ; Kinetics of CO2 hydrogenation on a K-promoted Fe catalyst. Ind Eng Chem Res ; Reaction kinetics over iron catalysts used for the Fischer-Tropsch synthesis. Can J Chem Eng ; Unsteady-state performance of heterogeneous catalytic reactions. Catal Rev Sci Eng ; Transient phenomena in three-way catalysis. Springer Science and Business Media Dordrecht, Catalytic process under Unsteady-State conditions. Stud Surf Sci Catal ; Modeling of surface intermediates under forced periodic conditions applied to CO2 methanation. Periodic operation of catalytic reactors-introduction and overview. Fischer-tropsch synthesis under periodic operation. Pulse-technique analysis of the kinetics of the fischer-tropsch reaction. Influence of forced cycling on the Fischer-Tropsch synthesis. Response to feed concentration step-changes. Response to feed concentration square-waves. Stankiewicz A, Kuczynski M. An industrial view on the dynamic operation of chemical converters, chemical engineering and processing. Study of unsteady-state operation of methanation by modeling and simulation. Chem Eng Technol ; Dynamic simulation of fixed-bed methanation reactors. Transient behaviour of an ammonia synthesis reactor. Chem Eng Sci ; Transient behaviour of an adiabatic fixed-bed methanatorâ€"I: Modeling and simulation in chemical engineering. Transient behaviour of an adiabatic fixed-bed methanatorâ€"II: Stability and dynamics of heterogeneous catalytic reaction systems. Int Chem Eng ; Chemical reactor design and control. Stankiewicz A, Eigenberger G. Dynamic modelling of multitubular catalytic reactors. An introduction to process flexibility part 2: Chem Eng Educ ; Commercial FT process aplications. Jaisathaporn P, Luyben W. Steady-state economic comparison of alternative tubular reactor systems. Betrachtungen des gesamtsystems im hinblick auf dynamik und prozessintegration teilprojekt 5. European network of transmission system operators for electricity. German transmission system operators. Fischerâ€"tropsch-synthesis with nitrogen-rich syngas: Appl Catal A Gen ; Iglesias Gonzalez M, Schaub G. Crossref About the article Published Online:

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Chapter 2 : Yurii Sh. Matros - Wikipedia

This book deals with catalytic processes under forced non-steady-state conditions. It demonstrates, both theoretically and practically, that forced non-steady-state processes are highly efficient compared with steady-state processes, and illustrates this with a wealth of practical examples.

Books[edit] Yu. Editor-in-chief of scientific work collections selected list [edit] Unsteady State Processes in Catalysis: Proceedings of International Conference, 5â€"8 June , Utrecht: Saint Petersburg, Russia, 28 Juneâ€"July Selected list of articles[edit] General[edit] Yurii Sh. Reverse-flow operation in fixed bed catalytic reactors. Reactors with a Fixed Bed of Catalyst, Kinet. VOC control[edit] J. Uhr, B Bullough, C. Conversion of a Regenerative Oxidizer into Catalytic Unit. Experimental Data and Reactor Simulation. Russian , 4, Theoretical Fundamentals of Chemical Technology , 18, SO2 oxidation[edit] V. Cancun, Mexico, Apr. Experience in Industry and Outlook. Houston, TX, , Frontiers in Chemical Engineering, Vol. Catalytic Process under Non-Steady Conditions. NOx reduction[edit] G. Environmental Protection, 6, ; 7, Calgary, Canada, Oct. Tekhnologii Theoretical Fundamentals of Chemical Technology , 22, Unsteady State Processes in Catalysis: Periodic Operation of Reactors, P. Van Impe, Chemical Engineering Science 62 â€" Masetti, Chemical Engineering Science 54 , pp. Bhatia, Chemical Engineering Science, Vol. Bunimovich, Tina Gilliland, Yurii Sh. Matros, and John D. Miller, November 1,

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Chapter 3 : Yurii Sh. Matros - Wikipedia

Works of the author with colleagues devoted to performance of catalytic processes in forced unsteady-state conditions in reactors with fixed bed of catalyst are briefly reviewed.

This book deals with catalytic processes under forced non-steady-state conditions. It demonstrates, both theoretically and practically, that forced non-steady-state processes are highly efficient compared with steady-state processes, and illustrates this with a wealth of practical examples. The first part of the book describes the theoretical and experimental basis of efficient processes, mathematical models of non-steady-state processes in reactors, influence of a non-steady-state catalyst surface, problems of optimization, the theory of a heat front in the fixed catalyst bed, and methods to create efficient cyclic regimes. The second part considers the following processes: The book will appeal to many readers: Franklin Feng Tao Language: This book presents both the fundamentals concepts and latest achievements of a field that is growing in importance since it represents a possible solution for global energy problems. It focuses on an atomic-level understanding of heterogeneous catalysis involved in important energy conversion processes. It presents a concise picture for the entire area of heterogeneous catalysis with vision at the atomic- and nano-scales, from synthesis, ex-situ and in-situ characterization, catalytic activity and selectivity, to mechanistic understanding based on experimental exploration and theoretical simulation. Addresses heterogeneous catalysis, one of the crucial technologies employed within the chemical and energy industries Presents the recent advances in the synthesis and characterization of nanocatalysts as well as a mechanistic understanding of catalysis at atomic level for important processes of energy conversion Provides a foundation for the potential design of revolutionarily new technical catalysts and thus the further development of efficient technologies for the global energy economy Includes both theoretical studies and experimental exploration Is useful as both a textbook for graduate and undergraduate students and a reference book for scientists and engineers in chemistry, materials science, and chemical engineering Author by: It is therefore essential that all chemists and chemical engineers have an understanding of the fundamental principles as well as the applications of heterogeneous catalysts. This book introduces the subject, starting at a basic level, and includes sections on adsorption and surface science, catalytic kinetics, experimental methods for preparing and studying heterogeneous catalysts, as well as some aspects of the design of industrial catalytic reactors. It ends with a chapter that covers a range of examples of important catalytic processes. The book leads the student to carrying out a series of "tasks" based on searches of the internet and also on the use of web-based search tools such as Scopus or Web of Science. The author has had over 40 years of experience in catalytic research as well as in lecturing on the principles of catalysis. He was for more than 20 years the Editor of Catalysis Today. Coverage of all aspects of catalysis in carefully organised text Inclusion of material on the historical development of the subject and the personalities involved All concepts illustrated by practical examples Inclusion of a wide range of problems and solutions, case studies, and supplementary web based material which will be regularly updated Author has over 40 years research experience of almost all covered subjects Provides companion materials webiste Author by: Elsevier Science Limited Format Available: This two-volume work provides an overview of the most common spectroscopic techniques which have been applied to reveal catalyst structures and surface characteristics in both model catalysts and those of industrial importance. A great amount of work on catalyst characterization using spectroscopic probes has been undertaken from both fundamental and applied perspectives. However, this general information is in urgent need of a critical revision. To undertake this task, a number of experts in the fields of structural and surface characterization of heterogeneous catalysts have contributed to this book. Part A provides an up-to-date review of the theoretical basis and applications of spectroscopic methods to identify catalyst structures photoelectron spectroscopy, ion scattering, infrared, extended X-ray absorption fine structure, Mossbauer. Part B concentrates on catalyst surfaces. The interaction of adsorbed molecules, mostly on heterogenous catalysts,

although some reference to model catalysts is also made, is discussed here.

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Chapter 4 : "Unsteady catalytic processes and sorption-catalytic technologies" by Andrey N Zagoruiko

This book deals with catalytic processes under forced non-steady-state conditions. It demonstrates, both theoretically and practically, that forced non-steady-state processes are highly efficient compared with steady-state processes, and illustrates this with examples.

Citations a, Progress in reverseprocess application to catalytic incineration problems, A bench scale study of reversed flow methanol synthesis, A comparison of forced feed cycling of the Fisher-Tropsch synthesis over iron and cobalt catalysts, A high gain observer for a class of uniformly observable systems, A new non-stationary process for the production of ethyl-acetate, A novel reverse flow strategy for ethylbenzene dehydrogenation in a packed bed reactor, A periodic flow reversal reactor: A simple observer for a class of nonlinear systems, A simple observer for nonlinear systems, application to bioreactors, A simplified design of reverse flow nonstationary reactor for low reactant concentration, Air purification by catalytic oxidation in an adiabatic packed bed reactor with periodic flow reversal. Air purification in a reverse-flow reactor: Analysis of an exothermic reversible reaction in a catalytic reactor with periodic flow reversal, Approximation by superpositions of sigmoidal function. Beeinflussung der effektiven gerschwindigkeit heterogen-katalytischer reaktionen durch aufgezuungene konzantrationsschwankungen, Behaviour of catalytic oxidation of carbon monoxide under cycling conditions, Bidirectional adiabatic synthesis gas reactor, Canonical design for nonlinear observers with linearizable error dynamics, Catalytic cleaning of polluted air: Catalytic combustion in a reactor with periodic flow reversal: Catalytic combustion of methane lean mixtures in a reverse flow reactor, Catalytic combustion of natural gas in a fixed bed reactor with flow reversal, Catalytic combustion of very lean mixtures in a reverse flow reactor using an internal electrical heater, Catalytic combustion with periodical flow reversal, Catalytic processes under unsteady-state conditions, Combustion of methane in a cyclic catalytic reactor, Complex dynamic behaviour of methanol synthesis in the ring reactor network, Composition cycling of an SO2 oxidation reactor, Concentration forcing in ammonia synthesis. Controlled cycling operation, Concentration forcing of catalytic surface rate process. Isothermal carbon monoxide oxidation over supported platinum, Control of an autothermal network of nonstationary catalytic reactors, Control of nonadiabatic packed bed reactor under periodic flow reversal, Control of volatile organic compounds by the catalytic reverse process, Conversion enhancement of exothermic reactions in unsteady-state ring reactor network. Conversion enhancement of exothermic reversible reactions in forced un steady-state catalytic reactors, in: Dependence of cooled reverse-flow reactor dynamic on reactor model, Design and control of a bench-scale reverse-flow reactor for VOC combustion, in: Development and design of a forced unsteady-state reactor through numerical simulation, Direct and indirect model based control using artificial neural networks, Dynamic neural networks in nonlinear predictive control an industrial application , Dynamic properties of the adiabatic tubular reactor with switch flow, Dynamic studies of acetylene hydrogenation on nickel catalysts, Dynamics and control of forced-unsteady-state catalytic combustors, in Nonlinear dynamics and control in process engineering. Effect of periodic operation on the selectivity of catalytic reactions, Effect of periodic process execution on radical polymerizations, Effect of temperature changes on a tubular heterogeneous catalytic reactor , Effect of the intraparticle mass transport limitations on temperature profiles and catalytic performance of the reverse-flow reactor for the partial oxidation of methane to synthesis gas, Effective models for packed-bed catalytic reactors, Efficient design and scale-up of reverse flow catalytic combustors, Enhancement of selectivity of oxidative reactions in forced unsteady-state reactors, in: Equivalence of one- and two-dimensional models for heat transfer processes in packed beds: Experimental and theoretical investigations on the influence of fluids, solids and interactions between them on thermal properties of porous rocks, Experimental studies of a consecutive-competitive reaction in steady state and forced periodic CSTRs, Experimental studies of the improvement of fixed-bed reactors by periodic operation â€" the catalytic oxidation of ethylene, Experimentelle untersuchung zum

periodischen reaktorbetrieb bei der heterogen katalysierten oxidehydrierung von isobutyraldehyd zu methacrolein, Fixed-bed reactors with periodic flow reversal: Flow reversal reactor for the catalytic combustion of lean methane mixtures, Forced unsteady state methanol synthesis in a reactor network, Gas dispersion in packed beds, Heat transfer characteristics of porous rocks, High gain estimation for nonlinear systems, Identification using feedforward networks. Importance of the wall effects in reverse flow reactors for catalytic combustion of methane lean mixtures, in: Improving selectivity and yield by conducting processes in a periodic fashion, Influence of composition modulation and product yield and selectivity in the partial oxidation of propylene over an antimony-tin oxide catalyst, Influence of forced feed composition cycling on catalytic methanol synthesis, Influence of forced feed composition cycling on the rate of ammonia synthesis over an industrial iron catalyst. Influence of the physical and chemical properties of the catalyst on the combustion of the fugitive emissions from coke ovens, Influence of the wall heat losses on the performance of a network of nonstationary catalytic burners, Limiting cases and approximate solutions for fixed-bed reactors with periodic flow reversal, Methanol synthesis in a forced unsteadystate reactor network, Methanol synthesis under periodic operation: Model predictive control of a catalytic reverse flow reactor, Model predictive control of chemical processes, Model predictive control with linear models, State of the art, The good, the bad, and the ugly, Theory and practice - a survey, Modeling and simulation of the reversed flow operation of fixed bed reactor for methanol synthesis, Modelling and simulation for adiabatic fixed bed reactor with flow reversal, Modelling of a tubular reactor with flow reversal, Modelling of reversed flow fixed bed reactor for catalytic decontamination of waste gases, Neural networks â€" A comprehensive foundation, Neural networks in chemistry and drug design, Nonlinear internal model control strategy for neural network models, Nonlinear model predictive control: A tutorial and survey, Nonlinear observers for local uniform observable systems, Nonlinear process control, Nonstationary catalytic destruction of lean waste gases in a network of burners and a reverse-flow reactor under non-adiabatic conditions, Nonstationary method for ammonia synthesis, Theoret. Numerical simulation of a periodic flow reversal reactor for sulfur dioxide oxidation, Observability and observers for nonlinear systems, Observer design for reverse flow reactor, On the influence of the catalyst physical properties on the stability of forced unsteady-state after-burners. On the properties of the forced unsteady-state ring reactor network. On the reduction of the formation of carbon deposits in forced unsteady-state catalytic reactors for the production of syngas, in:

Chapter 5 : DYNAMICS AND CONTROL OF FORCED UNSTEADY-STATE CATALYTIC REACTORS - C

[0be] - Catalytic Processes Under Unsteady State Conditions evaluation of heat transfer in a catalytic fixed bed reactor at high temperatures l m m jorge 1 r m m jorge 2 f fujii 3 and r giudici 3.

The microporous molecular structure of the zeolite ZSM-5 is exploited in catalysts used in refineries Zeolites are extruded as pellets for easy handling in catalytic reactors. Heterogeneous catalysts act in a different phase than the reactants. Most heterogeneous catalysts are solids that act on substrates in a liquid or gaseous reaction mixture. Diverse mechanisms for reactions on surfaces are known, depending on how the adsorption takes place Langmuir-Hinshelwood , Eley-Rideal , and Mars-van Krevelen. The smaller the catalyst particle size, the larger the surface area for a given mass of particles. A heterogeneous catalyst has active sites, which are the atoms or crystal faces where the reaction actually occurs. Depending on the mechanism, the active site may be either a planar exposed metal surface, a crystal edge with imperfect metal valence or a complicated combination of the two. Thus, not only most of the volume, but also most of the surface of a heterogeneous catalyst may be catalytically inactive. Finding out the nature of the active site requires technically challenging research. Thus, empirical research for finding out new metal combinations for catalysis continues. For example, in the Haber process , finely divided iron serves as a catalyst for the synthesis of ammonia from nitrogen and hydrogen. The reacting gases adsorb onto active sites on the iron particles. Once physically adsorbed, the reagents undergo chemisorption that results in dissociation into adsorbed atomic species, and new bonds between the resulting fragments form in part due to their close proximity. In this way the particularly strong triple bond in nitrogen is broken, which would be extremely uncommon in the gas phase due to its high activation energy. Thus, the activation energy of the overall reaction is lowered, and the rate of reaction increases. Heterogeneous catalysts are typically " supported ," which means that the catalyst is dispersed on a second material that enhances the effectiveness or minimizes their cost. Supports prevent or reduce agglomeration and sintering of the small catalyst particles, exposing more surface area, thus catalysts have a higher specific activity per gram on a support. Sometimes the support is merely a surface on which the catalyst is spread to increase the surface area. More often, the support and the catalyst interact, affecting the catalytic reaction. Supports are porous materials with a high surface area, most commonly alumina , zeolites or various kinds of activated carbon. Specialized supports include silicon dioxide , titanium dioxide , calcium carbonate , and barium sulfate. Electrocatalyst In the context of electrochemistry , specifically in fuel cell engineering, various metal-containing catalysts are used to enhance the rates of the half reactions that comprise the fuel cell. One common type of fuel cell electrocatalyst is based upon nanoparticles of platinum that are supported on slightly larger carbon particles. When in contact with one of the electrodes in a fuel cell, this platinum increases the rate of oxygen reduction either to water, or to hydroxide or hydrogen peroxide. Homogeneous catalysis Homogeneous catalysts function in the same phase as the reactants, but the mechanistic principles involved in heterogeneous catalysis are generally applicable. Typically homogeneous catalysts are dissolved in a solvent with the substrates. The aldehyde can be converted to various products such as alcohols or acids for e. For inorganic chemists, homogeneous catalysis is often synonymous with organometallic catalysts. Organocatalysis Whereas transition metals sometimes attract most of the attention in the study of catalysis, small organic molecules without metals can also exhibit catalytic properties, as is apparent from the fact that many enzymes lack transition metals. In the early s, these organocatalysts were considered "new generation" and are competitive to traditional metal -ion -containing catalysts. Organocatalysts are supposed to operate akin to metal-free enzymes utilizing, e. The discipline organocatalysis is divided in the application of covalent e. Photocatalysts[edit] Photocatalysis is the phenomenon where the catalyst can receive light such as visible light , be promoted to an excited state, and then undergo intersystem crossing with the starting material, returning to ground state without being consumed. The excited state of the starting material will then undergo reactions it ordinarily could not if directly illuminated. For example, singlet

oxygen is usually produced by photocatalysis. Photocatalysts are also the main ingredient in dye-sensitized solar cells. Enzymes and biocatalysts[edit] Main article: Most biocatalysts are enzymes, but other non-protein-based classes of biomolecules also exhibit catalytic properties including ribozymes , and synthetic deoxyribozymes. Several factors affect the activity of enzymes and other catalysts including temperature, pH, concentration of enzyme, substrate, and products. A particularly important reagent in enzymatic reactions is water, which is the product of many bond-forming reactions and a reactant in many bond-breaking processes. In biocatalysis , enzymes are employed to prepare many commodity chemicals including high-fructose corn syrup and acrylamide. Some monoclonal antibodies whose binding target is a stable molecule which resembles the transition state of a chemical reaction can function as weak catalysts for that chemical reaction by lowering its activation energy. Nanomaterial-based catalyst Nanocatalysts are nanomaterials with catalytic activities. They have been extensively explored for wide range of applications. Among them, the nanocatalysts with enzyme mimicking activities are collectively called as nanozymes.

Chapter 6 : SelectedWorks - Andrey N Zagoruiko

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Chapter 7 : Catalysis - Wikipedia

Catalytic processes that occur under conditions of the targeted unsteady state of the catalyst are considered. The highest efficiency of catalytic processes was found to be ensured by a controlled.

Chapter 8 : Industrial Physical Chemistry â€“ Chemical Plants and Industrial Chemistry Group

Catalytic processes under unsteady-state conditions, volume 43 â€" studies in surface science and catalysis, by Yu. Sh. Matros, , xiv + pages, Elsevier Science Publishers, Amsterdam & New York, U.S. $

Chapter 9 : "Unsteady catalytic processes and sorption-catalytic technologies" by Andrey N Zagoruiko

The opinion that performance of continuous catalytic processes under invariable conditions is highly efficient has gained great popularity, especially among chemical engineers. However, very often the optimal conditions of the process can be achieved with the so-called unsteady-state operation. The.