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DYNAMIC MODELLING, BIFURCATION AND CHAOTIC BEHAVIOUR OF GAS–SOLID CATALYTIC REACTORS

S.S.E.H. Elnashaie and S.S. Elshishini

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The discovery of chaos has considerably widened the scope of our knowledge regarding the dynamics of physical systems. Gas-solid catalytic reactors are important units in the petrochemical and petroleum refining industries and in the field of environmental protection. The knowledge required to understand and analyse the bifurcation, dynamics and chaotic behaviour of these reactors is widespread among many disciplines including chemical reaction engineering, chemistry, physics and pure and applied mathematics.

This book is the first to consolidate the progress in understanding the complex dynamics of catalytic reactors. It covers the most important aspects of the problem, which includes the formulation of the dynamic models for these systems, the basic dynamic, bifurcation and chaotic characteristics of the different types and configurations of these units, the industrial relevance of these complex dynamic phenomena, as well as the mathematical tools necessary for the detailed analysis of these complex dynamics.

This book is easy to read, and will therefore appeal to a wide spectrum of chemical engineering students and chemical engineers in academia and in industry; also students and researchers from other disciplines who are interested in the rich and fascinating complex dynamic characteristics of gas-solid catalytic reactors, will find it both interesting and useful.

About the authors

Professor Said S.E.H. Elnashaie is a Professor of Chemical Engineering at Cairo University and at King Saud University. He has been a visiting scholar at a number of European, North American and Australian universities and research centres. Professor Elnashaie has been active in research on the steady state and dynamic behaviour of gas-solid catalytic reactors for the last twenty-five years, and is a consultant to various petrochemical and petroleum refining companies. For the past ten years, he has been investigating the chaotic behaviour of chemical and biochemical systems. He has over 150 scientific publications in international journals and conferences.

Professor Shadia S. Elshishini joined the Chemistry department at King Saud University in 1981, and became a Professor of Chemical Engineering at Cairo University in 1991. She has over 80 publications in international journals and conferences.

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Dynamic Modelling Bifurcation And Chaotic Behaviour Of Gabolid Catalytic Reactors

S. S. E. H. Elnashaie

Dynamic Modelling Bifurcation And Chaotic Behaviour Of Gabolid Catalytic Reactors:

Dynamic Modelling, Bifurcation and Chaotic Behaviour of Gas-Solid Catalytic Reactors S. S. E. H. Elnashaie,1996-03-18

The Modelling and Dynamics of Catalysts and Fixed Bed Reactors Klavs Flemming Jensen,1980 Bifurcation Phenomena in Stirred Tanks and Catalytic Reactors Willis Harmon Ray,K. F. Jensen,K. K. Jensen,WISCONSIN UNIV-MADISON MATHEMATICS RESEARCH CENTER.,1980 A review of the present state of understanding of continuous stirred tank reactors is presented along with certain new results on bifurcation phenomena for catalytic surfaces A few examples are discussed which show repeated Hopf bifurcation complex oscillations and chaotic behaviour arising from a simple catalyst surface model The mathematical concepts brought to bear on this problem include static and Hopf bifurcation multiple and secondary bifurcation and singularity theory The features arising in the problems discussed here are thought to be common to a wide range of chemically reacting systems *The Dynamics and Stablilty of Fixed Bed Catalytic Reactors* Colin Ivan Adderley,1973 Various aspects of the behaviour of fixed bed reactors supporting highly exothermic reactions relevant to stable optimal design and control have been studied using detailed mathematical models In order to establish the form of the simplest basic structure two methods of describing radial heat transfer in two dimensional packed beds have been examined It is shown that a lumped parameter single phase heat transfer model which implicitly incorporates the heterogeneous structure can account not only for the radial heat flux associated with both the fluid and solid phases but is also the more appropriate formulation since it allows the important reaction rate limitations due to intraparticle mass transfer to be properly estimated Using this two dimensional heterogeneous dynamic model of the reactor it has been possible to evaluate a simpler one dimensional formulation It is shown that the latter gives an adequate description of the dynamic behaviour of the system provided that the overall heat transfer coefficient between the fluid and the coolant is suitably defined and may therefore be used for general studies of reactor performance Consideration has been given to the response of the reactor to sinusoidal perturbations of the inlet conditions It has been found that at certain frequencies of oscillation temperature runaway may develop before a safe quasi stationary state is reached A detailed examination of this behaviour has shown that in addition to the non linear effects the difference in the speeds of propagation of the concentration and temperature waves along the reactor as a result of the heterogeneity of the system is also very significant The effect of both cocurrent and countercurrent cooling of a single reactor tube has been examined The behaviour for perturbations in coolant temperature is similar to that for inlet temperature and indicates potential difficulties in the design of control systems A mathematical model of a multitubular reactor with crossflow cooling has been developed and used to identify some of the problems which may arise in these systems In particular considerable interaction between the individual reactor tubes occurs when significant conversion of the reactant takes place This causes tubes in different parts of the bundle to exhibit different behaviour and with countercurrent cooling this may give rise to multiple steady states due to the feedback of heat within the system A technique has been developed for predicting regions of parametric sensitivity and temperature runaway in heterogeneous fixed bed reactors The relationship between this form of instability and that due to multiple states of the catalyst pellet has been demonstrated Application of this method to both the design and control of a reactor is discussed and it is shown that it provides an insight as to the behaviour of the system since it makes possible the establishment of a relationship between local and global reactor stability and the operating variables Modelling, Simulation and Optimization of Industrial Fixed Bed Catalytic Reactors S.S.E.H. Elnashaie,2022-01-26 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 **Oscillating Heterogeneous Catalytic Systems** Marina M. Slin'ko,N.I. Jaeger,1994-08-26 A review of the mathematical concepts methods and tools needed for the analysis and the interpretation of complex phenomena associated with oscillating heterogeneous catalytic systems which in turn have much in common with dynamical systems studied in related fields such as physics and biology **Dynamic Behaviour of a Fixed-bed Catalytic Reactor with Catalyst Deactivation** ,1994 **Oscillations and chaos in chemical reactors** John Lester Hudson,1988 *Bifurcation, Instability and Chaos in Fluidized Bed Catalytic Reactors* Mohd Elbashir E. Abashar,1994 **Modeling and Simulation of Heterogeneous Catalytic Processes** ,2014-09-22 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 **Uncertainty Analysis and Robust Optimization of a Single Pore in a Heterogeneous Catalytic Flow Reactor System** Donovan Chaffart,2017 Catalytic systems are crucial to a wide number of chemical production processes and as a result there is significant demand to develop novel catalyst materials and to optimize existing catalytic reactor systems These optimization and design studies are most readily implemented using model based approaches which require less time and fewer resources than the alternative experimental based approaches The behaviour of a catalytic reactor system can be captured using multiscale modeling approaches that combine continuum transport equations with kinetic modeling approaches such as kinetic Monte Carlo kMC or the mean field MF approximation in order to model the relevant reactor phenomena on the length and time scales on which they occur These multiscale modeling approaches are able to accurately capture the reactor behaviour and can be readily implemented to perform robust optimization and process improvement studies on catalytic reaction systems The problem with multiscale based optimization of catalytic reactor systems however is that this is still an emerging field and there still remain a number of challenges that hinder these methods One such challenge involves the computational cost Multiscale modeling approaches can be computationally intensive which limit their application to model based optimization processes These computational burdens typically stem from the use of fine scale models that lack closed form expressions such as kMC A second common challenge involves model plant mismatch which can hinder the accuracy of the model This mismatch stems from uncertainty in the reaction pathways and from difficulties in obtaining the values of the system parameters from experimental results In addition the uncertainty in catalytic flow reactor systems can vary in space due to kinetic events not taken into consideration by the multiscale model such as non uniform catalyst deactivation due to poisoning and fouling mechanisms Failure to adequately account for model plant mismatch can result in substantial deviations from the predicted catalytic reactor performance and significant losses in reactor efficiency Furthermore uncertainty propagation techniques can be computationally intensive and can further increase the computational demands of the multiscale models Based on the above challenges the objective of this research is to develop and implement efficient strategies that study the effects of parametric uncertainty in key parameters on the performance of a multiscale single pore catalytic reactor system and subsequently to implement them to perform robust and dynamic optimization on the reactor system subject to uncertainty To this end low order series expansions such as Polynomial Chaos Expansion PCE and Power Series Expansion PSE were implemented in order to efficiently propagate parametric uncertainty through the multiscale reactor model These uncertainty propagation techniques were used to perform extensive uncertainty analyses on the catalytic reactor system in order to observe the impact of parametric uncertainty in various key system parameters on the catalyst reactor performance Subsequently these tools were implemented into robust optimization formulations that sought to maximize the reactor productivity and minimize the variability in the reactor performance due to uncertainty The results highlight the significant effect of parametric uncertainty on the reactor performance and illustrate how they can be accommodated for when performing robust optimization In order to assess the impact of spatially varying uncertainty due to catalyst deactivation on the catalytic reactor system the uncertainty propagation techniques were applied to evaluate and compare the effects of spatially constant and spatially varying uncertainty distributions To accommodate for the spatially varying uncertainty unique uncertainty descriptions were applied to each uncertain parameter at discretized points across the reactor length The uncertainty comparison was furthermore extended through application to robust optimization To reduce the computational cost statistical data driven models DDMs were identified to approximate the key statistical parameters mean variance and probabilistic bounds of the reactor output variability for each uncertainty distribution The DDMs were incorporated into robust optimization formulations that aimed to maximize the reactor productivity subject to uncertainty and minimize the uncertainty induced output variability The results demonstrate the impact of spatially varying parametric uncertainty on the catalytic reactor performance They also highlight the importance of its inclusion to adequately account for phenomena such as catalyst fouling in robust optimization and process improvement studies The dynamic behaviour of the catalytic reactor system was similarly assessed within this work to evaluate the effects of uncertainty on the reactor performance as it evolves in time and space For this study uncertainty analysis was performed on a transient multiscale catalytic reactor model subject to changes in the system temperature These results were used to formulate robust dynamic optimization studies to maximize the transient catalytic reactor behaviour These studies aimed to determine the optimal temperature trajectories that maximize the reactor s performance under uncertainty Dynamic optimization was also implemented to identify the optimal design and operating policies that allow the reactor under spatially varying uncertainty to meet targeted performance specifications within a level of confidence These studies illustrate the benefits of performing dynamic optimization to improve performance for multiscale process systems under uncertainty **The Dynamic Behaviour of a Fixed Bed Catalytic Reactor** Frederick Leder,1965 **Dynamic Modeling of Industrial Fixed Bed Catalytic Reactors** Omar Eugene Davis,Micheal Foley,Sydney Thomas,2005 Dynamics of Chemical Reactions and Reactors Ioannis George Kevrekidis,1985 Chemical and Catalytic Reactor Modeling American Chemical Society. Meeting,1984 *Unsteady State Processes in Catalysis* Yu S. Matros,1990-12 In the last decades the investigation methods of unsteady state catalytic processes have been widely developed by the response technique methods From this research emerged the realization that under unsteady state conditions and especially under artificially created ones it is possible to increase the productivity or selectivity of a catalyst or a catalytical process as a whole The scientific literature in this field is mostly theoretical and aims at structuring and analysing mathematical models of unsteady state catalytical processes In this book the theoretical and applied aspects of an efficiency of artificially created unsteady conditions in catalysis are discussed It contains the lectures from researchers from all over the world that were held during the International Conference Unsteady State Processes in Catalysis 5 8 June 1990 Novosibirsk USSR Topics include The problems of dynamics of a catalyst surface Kinetic models of unsteady processes Dynamics of chemical reactors Artificially created unsteady processes in a catalytic reactor **Towards Analytical Chaotic Evolutions in Brusselators** Albert C.J. Luo,Siyu Guo,2020-05-13 The Brusselator is a mathematical model for autocatalytic reaction which was proposed by Ilya Prigogine and his collaborators at the Universit Libre de Bruxelles The dynamics of the Brusselator gives an oscillating reaction mechanism for an autocatalytic oscillating chemical reaction The Brusselator is a slow fast oscillating chemical reaction system The traditional analytical methods cannot provide analytical solutions of such slow fast oscillating reaction and numerical simulations cannot provide a full picture of periodic evolutions in the Brusselator In this book the generalized harmonic balance methods are employed for analytical solutions of periodic evolutions of the Brusselator with a harmonic diffusion The bifurcation tree of period 1 motion to chaos of the Brusselator is presented through frequency amplitude characteristics which be measured in frequency domains Two main results presented in this book are analytical routes of periodical evolutions to chaos and independent period 2 1 evolution to chaos This book gives a better understanding of periodic evolutions to chaos in the slow fast varying Brusselator system and the bifurcation tree of period 1 evolution to chaos is clearly demonstrated which can help one understand routes of periodic evolutions to chaos in chemical reaction oscillators The slow fast varying systems extensively exist in biological systems and disease dynamical systems The methodology presented in this book can be used to investigate the slow fast varying oscillating motions in biological systems and disease dynamical systems for a better understanding of how infectious diseases spread **Dynamics of an Autocatalytic Reaction in a Membrane Reactor** Khalid Alhumaizi,1994 *Experimental Evaluation of Dynamic Models for a Fixed-bed Catalytic Reactor* John Arnold Hoiberg,1969 *Modelling Packed-tube Reactors with Data-based Transport Functions* Dennis F. Marr,1993

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