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Mathematical Modeling Rutherford Aris 1999-07-16 Mathematical modeling is the art and craft of building a system of equations that is both sufficiently complex to do justice to physical reality and sufficiently simple to give real insight into the situation. Mathematical Modeling: A Chemical Engineer's Perspective provides an elementary introduction to the craft by one of the century's most distinguished practitioners. Though the book is written from a chemical engineering viewpoint, the principles and pitfalls are common to all mathematical modeling of physical systems. Seventeen of the author's frequently cited papers are reprinted to illustrate applications to convective diffusion, formal chemical kinetics, heat and mass transfer, and the philosophy of modeling. An essay of acknowledgments, asides, and footnotes captures personal reflections on academic life and personalities. Describes pitfalls as well as principles of mathematical modeling Presents twenty examples of engineering problems Features seventeen reprinted papers Presents personal reflections on some of the great natural philosophers Emphasizes modeling procedures that precede extensive calculations *Dynamical Systems with Applications Using Mathematica®* Stephen Lynch 2017-10-12 This book provides an introduction to the theory of dynamical systems with the aid of the Mathematica® computer algebra package. The book has a very hands-on approach and takes the reader from basic theory to recently published research material. Emphasized throughout are numerous applications to biology, chemical kinetics, economics, electronics, epidemiology, nonlinear optics, mechanics, population dynamics, and neural networks. Theorems and proofs are kept to a minimum. The first section deals with continuous systems using ordinary differential equations, while the second part is devoted to the study of

discrete dynamical systems.
Nonlinear Differential Equations of Chemically Reacting Systems George R. Gavalas 2013-03-13 In recent years considerable interest has developed in the mathe matical analysis of chemically reacting systems both in the absence and in the presence of diffusion. Earlier work has been limited to simple problems amenable to closed form solutions, but now the computer permits the numerical solution of complex systems of nonlinear differ ential equations. The numerical approach provides quantitative infor mation, but for practical reasons it must be limited to a rather narrow range of the parameters of the problem. Consequently, it is desirable to obtain broader qualitative information about the solutions by in vestigating from a more fundamental mathematical point of view the structure of the differential equations. This theoretical approach can actually complement and guide the computational approach by narrow ing down trial and error procedures, pinpointing singularities and suggesting methods for handling them. The study of the structure of the differential equations may also clarify some physical principles and suggest new experiments. A serious limitation ofthe theoretical approach is that many of the results obtained, such as the sufficient conditions for the stability of the steady state, turn out to be very conservative. Thus the theoretical and computational approaches are best used to gether for the purpose of understanding, designing, and controlling chemically reacting systems. The present monograph is intended as a contribution to the theory of the differential equations describing chemically reacting systems.
Chemical Complexity via Simple Models Valeriy I. Bykov 2018-01-22 This book is focused on mathematical modelling of chemical kinetics. The authors present the classification of basic models of chemical kinetics, thermokinetics and macrokinetics, as well as their application for the most important chemical transformations, such as combustion and catalysis. Readers will find a detailed description and analysis of different mathematical instruments which can be applied for simulation of reaction dynamics.
Global Chemical Kinetics of Fossil Fuels Alan K. Burnham 2017-02-11 This book covers the origin and chemical structure of sedimentary organic matter, how that structure relates to appropriate chemical reaction models, how to obtain reaction data uncontaminated by heat and mass transfer, and how to convert that data into global kinetic models that extrapolate over wide temperature ranges. It also shows applications for in-situ and above-ground processing of oil shale, coal and other heavy fossil fuels. It is essential reading for anyone who wants to develop and apply reliable chemical kinetic models for natural petroleum formation and fossil fuel processing and is designed for course use in petroleum systems modelling. Problem sets, examples and case studies are included to aid in teaching and learning. It presents original work and contains an extensive reanalysis of data from the literature.
A Step by Step Approach to the Modeling of Chemical Engineering Processes Liliane Maria Ferrareso Lona 2017-12-15 This book treats modeling and simulation in a simple way, that builds on the existing knowledge and intuition of students. They will learn how to build a model and solve it using Excel. Most chemical engineering students feel a shiver down the spine when they see a set of complex mathematical equations generated from the modeling of a chemical engineering system. This is because they usually do not understand how to achieve this mathematical model, or they do not know how to solve the equations system without spending a lot of time and effort. Trying to understand how to generate a set of mathematical equations to represent a physical system (to model) and solve these equations (to simulate) is not a simple task. A model, most of the time, takes into account all phenomena studied during a Chemical Engineering course. In the same way, there is a multitude of numerical methods that can be used to solve the same set of equations generated from the modeling, and many different computational languages can be adopted to implement the numerical methods. As a consequence of this comprehensiveness and combinatorial explosion of possibilities, most books that deal with this subject are very extensive and embracing, making need for a lot of time and effort to go through this subject. It is expected that with this book the chemical engineering student and the future chemical engineer feel motivated to solve different practical problems involving chemical processes, knowing they can do that in an easy and fast way, with no need of expensive software.
Optimal Experimental Design for Non-Linear Models Christos P. Kitsos 2014-01-09 This book tackles the Optimal Non-Linear Experimental Design problem from an applications perspective. At the same time it offers extensive mathematical background material that avoids technicalities, making it accessible to non-mathematicians: Biologists, Medical Statisticians, Sociologists, Engineers, Chemists and Physicists will find new approaches to conducting their experiments. The book is recommended for Graduate Students and Researchers.
Multiple Time Scales Jeremiah U. Brackbill 2014-05-10 Multiple Time Scales presents various numerical methods for solving multiple-time-scale problems. The selection first elaborates on considerations on solving problems with multiple scales; problems with different time scales; and nonlinear normal-mode initialization of numerical weather prediction models. Discussions focus on analysis of observations, nonlinear analysis, systems of ordinary differential equations, and numerical methods for problems with multiple scales. The text then examines the diffusion-synthetic acceleration of transport iterations, with application to a radiation hydrodynamics problem and implicit methods in combustion and chemical kinetics modeling. The publication ponders on molecular dynamics and Monte Carlo simulations of rare events; direct implicit plasma simulation; orbit averaging and subcycling in particle simulation of plasmas; and hybrid and collisional implicit plasma simulation models. Topics include basic moment method, electron subcycling, gyroaveraged particle simulation, and the electromagnetic direct implicit method. The selection is a valuable reference for researchers interested in pursuing further research on the use of numerical methods in solving multiple-time-scale problems.
Nonlinear Phenomena in Chemical Dynamics C. Vidal 2012-12-06 An international conference. titled Nonlinear Phenomena in Chemical Dynamics was held in Bordeaux on September 7-11, 1981. The present volume contains the text of lectures and abstracts of posters presented during the meeting. This conference is part of a series of scientific multidisciplinary meetings in which chemistry is involved at various levels. Amongst the most recent ones let us mention Aachen 1979, Bielefeld 1979, New York 1979, Elmau 1981. In addition, this meeting is a direct extension of the first one that took place in Bordeaux in 1978 on the topic "Far from equilibrium: instabilities and structures," at the conclusions of which we could write (cf. Far fram Equilibrium, Springer Series in Synergetics, Vol. 3): "The three key words, far fram equilibriUm, instabilities and structuPes, best illustrate the new concepts which emerge from the description of the dynamics of various systems relevant to many different research areas. " The present proceedings show how much these remarks have remained true, even though substantial progress has been achieved during the three last years. To get a ,deeper experimental knowledge of open reacting systems, to model and simulate reaction-diffusion systems, to develop the mathematical theory of dynamical sys tems, these are the main direction~ in current investigations.
Scientific Computing in Chemical Engineering II Frerich Keil 2012-12-06 The application of modern methods in numerical mathematics on problems in chemical engineering is essential for designing, analyzing and running chemical processes and even entire plants. Scientific Computing in Chemical Engineering II gives the state of the art from the point of view of numerical mathematicians as well as that of engineers. The present volume as part of a two-volume edition covers topics such as the simulation of reactive flows, reaction engineering, reaction diffusion problems, and molecular properties. The volume is aimed at scientists, practitioners and graduate students in chemical engineering, industrial engineering and numerical mathematics.
Kinetics of Chemical Reactions Guy B. Marin 2018-12-07 This second, extended and updated edition presents the current state of kinetics of chemical reactions, combining basic knowledge with results recently obtained at the frontier of science. Special attention is paid to the problem of the chemical reaction complexity with theoretical and methodological concepts illustrated throughout by numerous examples taken from heterogeneous catalysis combustion and enzyme processes. Of great interest to graduate students in both chemistry and chemical engineering.
Modeling of Chemical Kinetics and Reactor Design A. Kayode Coker 2001 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

Coping with Complexity: Model Reduction and Data Analysis Alexander N. Gorban 2010-10-21 This volume contains the extended version of selected talks given at the international research workshop "Coping with Complexity: Model Reduction and Data Analysis", Ambleside, UK, August 31 – September 4, 2009. The book is deliberately broad in scope and aims at promoting new ideas and methodological perspectives. The topics of the chapters range from theoretical analysis of complex and multiscale mathematical models to applications in e.g., fluid dynamics and chemical kinetics.

Computer-Aided Modeling of Reactive Systems Warren E. Stewart 2008-03-17 Learn to apply modeling and parameter estimation tools and strategies to chemicalprocesses using your personal computer This book introduces readers to powerful parameter estimation and computational methods for modeling complex chemical reactions and reaction processes. It presents useful mathematical models, numerical methods for solving them, and statistical methods for testing and discriminating candidate models with experimental data. Topics covered include: Chemical reaction models Chemical reactor models Probability and statistics Bayesian estimation Process modeling with single-response data Process modeling with multi-response data Computer software (Athena Visual Studio) is available via a related Web site http://www.athenavisual.com enabling readers to carry out parameter estimation based on their data and to carry out process modeling using these parameters. As an aid to the reader, an appendix of example problems and solutions is provided. Computer-Aided Modeling of Reactive Systems is an ideal supplemental text for advanced undergraduates and graduate students in chemical engineering courses, while it also serves as a valuable resource for practitioners in industry who want to keep up to date on the most current tools and strategies available.

Nonlinear Computer Modeling of Chemical and Biochemical Data James F. Rusling 1996-02-05 Assuming only background knowledge of algebra and elementary calculus, and access to a modern personal computer, Nonlinear Computer Modeling of Chemical and Biochemical Data presents the fundamental basis and procedures of data modeling by computer using nonlinear regression analysis. Bypassing the need for intermediary analytical stages, this method allows for rapid analysis of highly complex processes, thereby enabling reliable information to be extracted from raw experimental data. By far the greater part of the book is devoted to selected applications of computer modeling to various experiments used in chemical and biochemical research. The discussions include a short review of principles and models for each technique, examples of computer modeling for real and theoretical data sets, and examples from the literature specific to each instrumental technique. The book also offers detailed tutorial on how to construct suitable models and a score list of appropriate mathematics software packages.

Scientific Computation with Automatic Result Verification Ulrich Kulisch 2012-12-06 Scientific Computation with Result Verification has been a persevering research topic at the Institute for Applied Mathematics of Karlsruhe University for many years. A good number of meetings have been devoted to this area. The latest of these meetings was held from 30 September to 2 October, 1987, in Karlsruhe; it was co-sponsored by the GAMM Committee on "Computer Arithmetic and Scientific Computation". -- This volume combines edited versions of selected papers presented at this confer ence, including a few which were presented at a similar meeting one year earlier. The selection was made on the basis of relevance to the topic chosen for this volume. All papers are original contributions. In an appendix, we have supplied a short account of the Fortran-SC language which permits the programming of algorithms with result verification in a natural manner. The editors hope that the publication of this material as a Supplementum of Computing will further stimulate the interest of the scientific community in this important tool for Scientific Computation. In particular, we would like to make application scientists aware of its potential. The papers in the second chapter of this volume should convince them that automatic result verification may help them to design more reliable software for their particular tasks. We wish to thank all contributors for adapting their manuscripts to the goals of this volume. We are also grateful to the Publisher, Springer-Verlag of Vienna, for an efficient and quick production.

Quasichemical Models of Multicomponent Nonlinear Diffusion Hafiz Abdul Wahab 2011 Diffusion preserves positivity of concentrations, therefore, multicomponent diffusion should be nonlinear if there exist non-diagonal terms. The vast variety of nonlinear multicomponent diffusion equations should be ordered and special tools are necessary to provide systematic construction of the nonlinear diffusion equations for multicomponent mixtures with significant interaction between components. We develop an approach to nonlinear multicomponent diffusion based on the idea of reaction mechanism borrowed from chemical kinetics. Chemical kinetics gave rise to the very seminal tools for the modelling of processes. This is the stoichiometric algebra supplemented by the simple kinetic law. The results of this invention are now applied in many areas of science, from particle physics to sociology. In our work we extend the area of applications onto nonlinear multicomponent diffusion. We demonstrate, how the mechanism based approach to multicomponent diffusion can be included into the general thermodynamic framework, and prove the corresponding dissipation inequalities. To satisfy the thermodynamic restrictions, the kinetic law of an elementary process cannot have an arbitrary form. For the general kinetic law (the generalized Mass Action Law), additional conditions are proved. The cell-jump formalism gives an intuitively clear representation of the elementary transport processes and, at the same time, produces kinetic finite elements, a tool for numerical simulation.

Spatial Inhomogeneities and Transient Behaviour in Chemical Kinetics Peter Gray 1990 The results of an International Conference on [title] held in Brussels, Belgium, Aug./Sept. 1987, these papers deal with self-organization and nonlinear dynamics in chemistry, giving the results of recent experiments and bringing new emphasis on spatial inhomogeneities and dynamical phenomena in con"

Stochastic Chemical Kinetics Péter Érdi 2014-05-06 This volume reviews the theory and simulation methods of stochastic kinetics by integrating historical and recent perspectives, presents applications, mostly in the context of systems biology and also in combustion theory. In recent years, due to the development in experimental techniques, such as optical imaging, single cell analysis, and fluorescence spectroscopy, biochemical kinetic data inside single living cells have increasingly been available. The emergence of systems biology brought renaissance in the application of stochastic kinetic methods.

Chemical Instabilities G. Nicolis 2012-12-06 On March 14-18, 1983 a workshop on "Chemical Instabilities: Applications in Chemistry, Engineering, Geology, and Materials Science" was held in Austin, Texas, U.S.A. It was organized jointly by the University of Texas at Austin and the Universite Libre de Bruxelles and sponsored qy NATO, NSF, the University of Texas at Austin, the International Solvay Institutes and the Ex xon Corporation. The present Volume includes most of the material of the in vited lectures delivered in the workshop as well as material from some posters, whose content was directly related to the themes of the invited lectures. In ,recent years, problems related to the stability and the nonlinear dynamics of nonequilibrium systems invaded a great num ber of fields ranging from abstract mathematics to biology. One of the most striking aspects of this development is that subjects reputed to be "classical" and "well-established" like chemistry, turned out to give rise to a rich variety of phenomena leading to multiple steady states and hysteresis, oscillatory behavior in time, spatial patterns, or propagating wave fronts. The primary objective of the workshop was to bring together researchers actively engaged in fields in which instabilities and nonlinear phenomena similar to those observed in chemistry are of current and primary concern : chemical engineering (especially surface catalysis), combustion (dynamics of ignition, flame sta bili t;y), interfaces (emulsification, dendritic growth), geology (regularly repeated patterns of mineralization 1n a variety of spabe scales), and materials science (dynamical solidification, behavior of matter under irradiation).

Nonlinear Chemical Kinetics 2002 This discussion stimulates interactions between the nonlinear kinetic community and more traditional physical chemists.

Model Reduction and Coarse-Graining Approaches for Multiscale Phenomena Alexander N. Gorban 2006-09-22 Model reduction and coarse-graining are important in many areas of science and engineering. How does a system with many degrees of freedom become one with fewer? How can a reversible micro-description be adapted to the dissipative macroscopic model? These crucial questions, as well as many other related problems, are discussed in this book. All contributions are by experts whose specialities span a wide range of fields within science and

engineering.
Nonlinear Modelling of Chemical Kinetics for the Acid Mine Drainage Problem and Related Physical Topics J. A. Tuszynski 1993
Invariant Manifolds for Physical and Chemical Kinetics Alexander N. Gorban 2005-02-01 By bringing together various ideas and methods for extracting the slow manifolds, the authors show that it is possible to establish a more macroscopic description in nonequilibrium systems. The book treats slowness as stability. A unifying geometrical viewpoint of the thermodynamics of slow and fast motion enables the development of reduction techniques, both analytical and numerical. Examples considered in the book range from the Boltzmann kinetic equation and hydrodynamics to the Fokker-Planck equations of polymer dynamics and models of chemical kinetics describing oxidation reactions. Special chapters are devoted to model reduction in classical statistical dynamics, natural selection, and exact solutions for slow hydrodynamic manifolds. The book will be a major reference source for both theoretical and applied model reduction. Intended primarily as a postgraduate-level text in nonequilibrium kinetics and model reduction, it will also be valuable to PhD students and researchers in applied mathematics, physics and various fields of engineering.
An Introduction to Scientific Computing Ionut Danaila 2007-12-03 This book demonstrates scientific computing by presenting twelve computational projects in several disciplines including Fluid Mechanics, Thermal Science, Computer Aided Design, Signal Processing and more. Each follows typical steps of scientific computing, from physical and mathematical description, to numerical formulation and programming and critical discussion of results. The text teaches practical methods not usually available in basic textbooks: numerical checking of accuracy, choice of boundary conditions, effective solving of linear systems, comparison to exact solutions and more. The final section of each project contains the solutions to proposed exercises and guides the reader in using the MATLAB scripts available online.
Mathematical Models of Chemical Reactions Péter Érdi 1989
Modeling and Simulation of Turbulent Combustion Santanu De 2017-12-12 This book presents a comprehensive review of state-of-the-art models for turbulent combustion, with special emphasis on the theory, development and applications of combustion models in practical combustion systems. It simplifies the complex multi-scale and nonlinear interaction between chemistry and turbulence to allow a broader audience to understand the modeling and numerical simulations of turbulent combustion, which remains at the forefront of research due to its industrial relevance. Further, the book provides a holistic view by covering a diverse range of basic and advanced topics—from the fundamentals of turbulence–chemistry interactions, role of high-performance computing in combustion simulations, and optimization and reduction techniques for chemical kinetics, to state-of-the-art modeling strategies for turbulent premixed and nonpremixed combustion and their applications in engineering contexts.
Chemical Oscillations and Instabilities Peter Gray 1994 Scientists in many fields are now expressing considerable interest in non-linearity and the ideas of oscillations and chaos. Chemical reactions provide perfect examples of these phenomena, as oscillating reactions, explosions, ignition, travelling waves, patterns, quasiperiodicity, and chaosare all features of chemical kinetics.Now available in paperback, this book introduces non-linear phenomena in chemical kinetics using simple model schemes. These models involve chemical feedback, such as chain branching, autocatalysis, and self-heating. The emphasis is on physical and pictorial representation, and on identifying thosegross features which are essential. The experimental conditions under which such behaviour will occur can be predicted using simple mathematical recipes, and these are also included.The first part of the book begins with a discussion of long-lived oscillations for autocatalytic or exothermic reactions in closed vessels. Stationary states, bistability, and oscillations in continuous flow reactors and diffusion cells are then considered. This is followed by chemical wavepropagation and by pattern selection and oscillations. Complex oscillations, quasiperiodicity, and chemical chaos, either forced or spontaneous, are introduced. Part 2 deals with real experimental systems, describing observed experimental behaviour and its interpretation in terms of the underlyingchemical mechanisms or simplified models. The Belousov-Zhabotinskii reactions is discussed in some detail as the most extensively studied system, and the behaviour of important gas phase reactions is presented.
Discrete and Topological Models in Molecular Biology Nataša Jonoska 2013-12-23 Theoretical tools and insights from discrete mathematics, theoretical computer science, and topology now play essential roles in our understanding of vital biomolecular processes. The related methods are now employed in various fields of mathematical biology as instruments to "zoom in" on processes at a molecular level. This book contains expository chapters on how contemporary models from discrete mathematics – in domains such as algebra, combinatorics, and graph and knot theories – can provide perspective on biomolecular problems ranging from data analysis, molecular and gene arrangements and structures, and knotted DNA embeddings via spatial graph models to the dynamics and kinetics of molecular interactions. The contributing authors are among the leading scientists in this field and the book is a reference for researchers in mathematics and theoretical computer science who are engaged with modeling molecular and biological phenomena using discrete methods. It may also serve as a guide and supplement for graduate courses in mathematical biology or bioinformatics, introducing nontraditional aspects of mathematical biology.
Modelling of Chemical Reaction Systems K.H. Ebert 2012-12-06 For rather a long time numerical results in chemical kinetics could only be obtained for very simple chemical reactions, most of which were of minor practi ca 1 importance. The avail abil ity of fast computers has provi ded new opportunities for developments in chemical kinetics. Chemical systems of practical interest are usually very complicated. They consi st of a great number of different el ementary chemi cal reacti ons, mostly with rate constants differi ng by many orders of magni tude, frequently with surface reacti on steps and often wi th transport processes. The deri vati on of a 'true' chemical mechani sm can be extremely cumbersome. Mostly this work is done by setting up 'reaction models' which are im proved step by step in comparison with precise experimental data. At this early stage mathematics is involved, which may al ready be rather complicated. Mathematical methods such as pertubation theory, graph theory, sensitivity analysis or numerical integration are necessary for the derivation and application of optimal chemical reaction models. Most theoretical work aimed at improving the mathematical methods was done on chemical reactions which mostly were of little practical im portance. Chemi cal engi neers, who evi dently k now well how important the chemical model s and their dynamics are for reactor desi gn, have al so to be convinced not only on the theoretical work but also on its practical applic abil ity.
Dynamical Systems with Applications using MapleTM Stephen Lynch 2009-12-23 Excellent reviews of the first edition (Mathematical Reviews, SIAM, Reviews, UK Nonlinear News, The Maple Reporter) New edition has been thoroughly updated and expanded to include more applications, examples, and exercises, all with solutions Two new chapters on neural networks and simulation have also been added Wide variety of topics covered with applications to many fields, including mechanical systems, chemical kinetics, economics, population dynamics, nonlinear optics, and materials science Accessible to a broad, interdisciplinary audience of readers with a general mathematical background, including senior undergraduates, graduate students, and working scientists in various branches of applied mathematics, the natural sciences, and engineering A hands-on approach is used with Maple as a pedagogical tool throughout; Maple worksheet files are listed at the end of each chapter, and along with commands, programs, and output may be viewed in color at the author’s website with additional applications and further links of interest at Maplesoft’s Application Center
Analysis of Kinetic Reaction Mechanisms Tamás Turányi 2014-12-29 Chemical processes in many fields of science and technology, including combustion, atmospheric chemistry, environmental modelling, process engineering, and systems biology, can be described by detailed reaction mechanisms consisting of numerous reaction steps. This book describes methods for the analysis of reaction mechanisms that are applicable in all these fields. Topics addressed include: how sensitivity and uncertainty analyses allow the calculation of the overall uncertainty of simulation results and the identification of the most important input parameters, the ways in which mechanisms can be reduced without losing important kinetic and dynamic detail, and the application of reduced models for more accurate engineering optimizations. This monograph is invaluable for researchers and engineers dealing with detailed reaction mechanisms, but is also useful for graduate students of related courses in chemistry, mechanical engineering, energy and environmental science and biology.
Sequential Design of Experiments for Nonlinear Models G. E. P. BOX 1963 To engineers, basic mechanism studies are of interest principally because a deeper understanding makes it possible to cope with engineering design problems in a more intelligent and useful manner than would be possible if the mechanism were entirely unknown. Such

mechanism studies consist essentially of two steps: (i) establishing an adequate form for the theoretical model and then (ii) determining precisely the values of its parameters. In this paper it is supposed that step (i) has been accomplished and the form of the theoretical model is therefore known. The problem which confronts the experimenter now is the evaluation of the physical parameters (e.g., rate constants in chemical kinetics examples). The purpose of this paper is to consider the problem of generation of data, i.e., the statistical design of experiments.
Dynamic Model Development: Methods, Theory and Applications S. Macchietto 2003-08-04 Detailed mathematical models are increasingly being used by companies to gain competitive advantage through such applications as model-based process design, control and optimization. Thus, building various types of high quality models for processing systems has become a key activity in Process Engineering. This activity involves the use of several methods and techniques including model solution techniques, nonlinear systems identification, model verification and validation, and optimal design of experiments just to name a few. In turn, several issues and open-ended problems arise within these methods, including, for instance, use of higher-order information in establishing parameter estimates, establishing metrics for model credibility, and extending experiment design to the dynamic situation. The material covered in this book is aimed at allowing easier development and full use of detailed and high fidelity models. Potential applications of these techniques in all engineering disciplines are abundant, including applications in chemical kinetics and reaction mechanism elucidation, polymer reaction engineering, and physical properties estimation. On the academic side, the book will serve to generate research ideas. Contains wide coverage of statistical methods applied to process modelling Serves as a recent compilation of dynamic model building tools Presents several examples of applying advanced statistical and modelling methods to real process systems problems
Design of Experiments in Nonlinear Models Luc Pronzato 2013-04-10 Design of Experiments in Nonlinear Models: Asymptotic Normality, Optimality Criteria and Small-Sample Properties provides a comprehensive coverage of the various aspects of experimental design for nonlinear models. The book contains original contributions to the theory of optimal experiments that will interest students and researchers in the field. Practitionners motivated by applications will find valuable tools to help them designing their experiments. The first three chapters expose the connections between the asymptotic properties of estimators in parametric models and experimental design, with more emphasis than usual on some particular aspects like the estimation of a nonlinear function of the model parameters, models with heteroscedastic errors, etc. Classical optimality criteria based on those asymptotic properties are then presented thoroughly in a special chapter. Three chapters are dedicated to specific issues raised by nonlinear models. The construction of design criteria derived from non-asymptotic considerations (small-sample situation) is detailed. The connection between design and identifiability/estimability issues is investigated. Several approaches are presented to face the problem caused by the dependence of an optimal design on the value of the parameters to be estimated. A survey of algorithmic methods for the construction of optimal designs is provided.
Chemical Kinetics, Stochastic Processes, and Irreversible Thermodynamics Moisés Santillán 2014-06-27 This book brings theories in nonlinear dynamics, stochastic processes, irreversible thermodynamics, physical chemistry and biochemistry together in an introductory but formal and comprehensive manner. Coupled with examples, the theories are developed stepwise, starting with the simplest concepts and building upon them into a more general framework. Furthermore, each new mathematical derivation is immediately applied to one or more biological systems. The last chapters focus on applying mathematical and physical techniques to study systems such as: gene regulatory networks and molecular motors. The target audience of this book are mainly final year undergraduate and graduate students with a solid mathematical background (physicists, mathematicians and engineers), as well as with basic notions of biochemistry and cellular biology. This book can also be useful to students with a biological background who are interested in mathematical modeling and have a working knowledge of calculus, differential equations and a basic understanding of probability theory.
Chaos in Chemistry and Biochemistry Richard J Field 1993-03-31 True deterministic chaos is characterized by unpredictable, apparently random motion in a dynamical system completely described by a deterministic dynamic law, usually a nonlinear differential equation, with no stochastic component. The inability to predict future behavior of a chaotic system occurs because trajectories evolving from arbitrarily close initial conditions diverge. Chaos is universal as it may arise in any system governed by one of a class of quite common, suitable nonlinear dynamic laws. This book discusses both the experimental observation and theoretical interpretation of chaos in chemical and biochemical systems. Examples are drawn from the Belousov-Zhabotinsky reaction, surface reactions, electrochemical reactions, enzyme reactions, and periodically perturbed oscillating systems. Contents:Mathematics of Chaos in Perturbed Oscillators (W R Derrick)Dynamical Systems Theory Illustrated: Chaotic Behavior in the Belousov-Zhabotinsky Reaction (J-C Roux)Modeling and Interpretation of Chaos in the Belousov-Zhabotinsky Reaction (L Györgyi & R J Field)Chaos in Forced and Coupled Chemical Oscillators and Excitators (M Marek & I Schreiber)Chaos in Electrochemical Systems (J L Hudson)Chaos in Surface-Catalyzed Reactions (M Eiswirth)Chaos in Biochemical Systems: The Peroxidase Reaction as a Case Study (R Larter et al.)A New Theoretical Approach to the Description of Physico-Chemical Reaction Dynamics with Chaotic Behavior (V Gontar)From Periodicity Behavior to Chaos in Biochemical Systems (A Goldbeter) Readership: Research workers at undergraduates and higher levels. keywords:
Nonlinear Modelling of Chemical Kinetics for the Acid Mine Drainage Problem and Related Physical Topics Jacek Adam Tuszyński 1994*
Advanced Chemical Kinetics Muhammad Akhyar Farrukh 2018-02-21 The book on Advanced Chemical Kinetics gives insight into different aspects of chemical reactions both at the bulk and nanoscale level and covers topics from basic to high class. This book has been divided into three sections: (i) "Kinetics Modeling and Mechanism," (ii) "Kinetics of Nanomaterials," and (iii) "Kinetics Techniques." The first section consists of six chapters with a variety of topics like activation energy and complexity of chemical reactions; the measurement of reaction routes; mathematical modeling analysis and simulation of enzyme kinetics; mechanisms of homogeneous charge compression ignition combustion for the fuels; photophysical processes and photochemical changes; the mechanism of hydroxyl radical, hydrate electron, and hydrogen atom; and acceptorless alcohol dehydrogenation. The understanding of the kinetics of nanomaterials, to bridge the knowledge gap, is presented in the second section. The third section highlights an overview of experimental techniques used to study the mechanism of reactions.
MODA4 — Advances in Model-Oriented Data Analysis Christos P. Kitsos 2013-06-29 This volume is the proceedings of the 4th International Workshop on Model-Oriented Data Analysis. This series of events originated in 1987 at a meeting in Eisenach, that successfully brought together scientists from numerous countries of the 'East ' and 'West'. Now that this distinction is obsolete dialogue has been greatly facilitated, providing opportunities for this dialogue, however, is as vital as ever. The present meeting at Spetses, Greece from 5th to 9th of June 1995 again assembles statisticians from all over the world as this book documents. The hospitality offered by the University of Economics of Athens and the Korgialenios School made it possible to organize this workshop. The editors are also grateful to Intracom (Greece), the Ionian Bank and the Procter & Gamble Company (USA) for their generous support. We would particularly like to mention Dr. Michael Meredith, who being our contact person at Procter & Gamble, enabled us to publish these proceedings. Further thanks go to Dr. Peter Schuster from Physica Verlag Heidelberg for his continuing support of the project. The contributions to this volume were carefully selected from the submissions by the editors after a one stage refereeing process. We would like to thank the members of the MODA committee, A.C. Atkinson, R.D. Cook, V.V. Fedorov, P.Hackl, H. Lauter, B.Torsney, LN. Vuchkov, H.P.Wynn,and A.A. Zhigljavsky, who not only defined the main topics of the workshop, but also served as the referees.