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Chemistry of Hydrocarbon Combustion Combustion Chemistry Low-temperature Combustion and Autoignition *Combustion* **Introduction to Physics and Chemistry of Combustion** *Combustion* **Gas-Phase Combustion Chemistry Fundamentals and Technology of Combustion** Combustion and Pollution Control in Heating Systems **Solid Propellant Chemistry Combustion and Motor Interior Ballistics 1999 Combustion Combustion and Flames** *Major Research Topics in Combustion Fundamentals of Combustion Processes* **Mathematical Modeling in Combustion and Related Topics Combustion Chemistry Pulverized-Coal Combustion and Gasification Chemistry of Hydrocarbon Combustion Flame and Combustion Physical and Chemical Aspects of Combustion** *Combustion Chemistry and the Carbon Neutral Future* **The Chemistry of Propellants** *Coal Combustion and Gasification* **Introduction to Combustion Phenomena** *Chemistry of Engine Combustion Deposits* **Combustion** Chemical Kinetics in Combustion and Reactive Flows: Modeling Tools and Applications Thermal Decomposition and Combustion of Explosives and Propellants **Combustion** Chemically Reacting Flow **Pollutants from Combustion** Combustion **Flame and Combustion** Mixture Formation in Internal Combustion Engines Nonequilibrium Processes in Physics and Chemistry **Turbulent Combustion Reacting Flows Advanced Combustion Science** Chemical Physics of Pyrolysis, Combustion, and Oxidation *Modeling Engine Spray and Combustion Processes*

Fundamentals and Technology of Combustion contains brief descriptions of combustion fundamental processes, followed by an extensive survey of the combustion research technology. It also includes mathematical combustion modeling of the processes covering mainly premixed and diffusion flames, where many chemical and physical processes compete in complex ways, for both laminar and turbulent flows. The combustion chemistry models that validate experimental data for different fuels are sufficiently accurate to allow confident predictions of the flame characteristics. This illustrates a unique bridge between combustion fundamentals and combustion technology, which provides a valuable technical reference for many engineers and scientists. Moreover, the book gives the reader sufficient background of basic engineering sciences such as chemistry, thermodynamics, heat transfer and fluid mechanics. The combustion research and mathematical models fit between small-scale laboratory burner flames, and large-scale industrial boilers, furnaces and combustion chambers. The materials have been collected from previous relevant research and some selected papers of the authors and co-workers, which have been presented mainly in different refereed journals, international conferences and symposia, thus providing a comprehensive collection. Furthermore, the book includes some of the many recent general correlations for the characteristics of laminar, turbulent, premixed and diffusion flames in an easily usable form. The authors believe that further progress in optimizing combustion performance and reducing polluting emissions can only be treated through understanding of combustion chemistry. The combustion of fossil fuels remains a key technology for the foreseeable future. It is therefore important that we understand the mechanisms of combustion and, in particular, the role of turbulence within this process. Combustion always takes place within a turbulent flow field for two reasons: turbulence increases the mixing process and enhances combustion, but at the same time combustion releases heat which generates flow instability through buoyancy, thus enhancing the transition to turbulence. The four chapters of this book present a thorough introduction to the field of turbulent combustion. After an overview of modeling approaches, the three remaining chapters consider the three distinct cases of premixed, non-premixed, and partially premixed combustion, respectively. This book will be of value to researchers and students of engineering and applied mathematics by demonstrating the current theories of turbulent combustion within a unified presentation of the field. Complex chemically reacting flow simulations are commonly employed to develop quantitative understanding and to optimize reaction conditions in systems such as combustion, catalysis, chemical vapor deposition, and other chemical processes. Although reaction conditions, geometries, and fluid flow can vary widely among the applications of chemically reacting flows, all applications share a need for accurate, detailed descriptions of the chemical kinetics occurring in the gas-phase or on reactive surfaces. Chemically Reacting Flow: Theory and Practice combines fundamental concepts in fluid mechanics and physical chemistry, assisting the student and practicing researcher in developing analytical and simulation skills that are useful and extendable for solving real-world engineering problems. The first several chapters introduce transport processes, primarily from a fluid-mechanics point of view, incorporating computational simulation from the outset. The middle section targets physical chemistry topics that are required to develop chemically reacting flow simulations, such as chemical thermodynamics, molecular transport, chemical rate theories, and reaction mechanisms. The final chapters deal with complex chemically reacting flow simulations, emphasizing combustion and materials processing. Among other features, Chemically Reacting Flow: Theory and Practice: -Advances a comprehensive approach to interweaving the fundamentals of chemical kinetics and fluid mechanics -Embraces computational simulation, equipping the reader with effective, practical tools for solving real-world problems -Emphasizes physical fundamentals, enabling the analyst to understand how reacting flow simulations achieve their results -Provides a valuable resource for scientists and engineers who use Chemkin or similar software Computer simulation of reactive systems is highly effective in the development, enhancement, and optimization of chemical processes. Chemically Reacting Flow helps prepare both students and professionals to take practical advantage of this powerful capability. A systematic control of mixture formation with modern high-pressure injection systems enables us to achieve considerable improvements of the combustion pr- ess in terms of reduced fuel consumption and engine-out raw emissions. However, because of the growing number of free parameters due to more flexible injection systems, variable valve trains, the application of different combustion concepts within different regions of the engine map, etc., the prediction of spray and m- ture formation becomes increasingly complex. For this reason, the optimization of the in-cylinder processes using 3D computational fluid dynamics (CFD) becomes increasingly important. In these CFD codes, the detailed modeling of spray and mixture formation is a prerequisite for the correct calculation of the subsequent processes like ignition, combustion and formation of emissions. Although such simulation tools can be viewed as standard tools today, the predictive quality of the sub-models is c- stantly enhanced by a more accurate and detailed modeling of the relevant pr- esses, and by the inclusion of new important mechanisms and effects that come along with the development of new injection systems and have not been cons- ered so far. In this book the most widely used mathematical models for the simulation of spray and mixture formation in 3D CFD calculations are described and discussed. In order to give the reader an introduction into the complex processes, the book starts with a description of the fundamental mechanisms and categories of fuel - jection, spray break-up, and mixture formation in internal combustion engines. The use of coal is required to help satisfy the world's energy needs. Yet coal is a difficult fossil fuel to consume efficiently and cleanly. We believe that its clean and efficient use can be increased through improved technology based on a thorough understanding of fundamental physical and chemical processes that occur during consumption. The principal objective of this book is to provide a current summary of this technology. The past technology for describing and analyzing coal furnaces and combus tors has relied largely on empirical inputs for the complex flow and chemical reactions that occur while more formally treating the heat-transfer effects. GrOWing concern over control of combustion-generated air pollutants revealed a lack of understanding of the relevant fundamental physical and chemical mechanisms. Recent technical advances in computer speed and storage capacity, and in numerical prediction of recirculating turbulent flows, two-phase flows, and flows with chemical reaction have opened new opportunities for describing and modeling such complex combustion systems in greater detail. We believe that most of the requisite component models to permit a more fundamental description of coal combustion processes are available. At the same time there is worldwide interest in the use of coal, and progress in modeling of coal reaction processes has been steady. The book is intended to serve as a primer to combustion. It has been the author's experience that too many scientists with interests in com bustion phenomena have very limited knowledge of the field as a whole. For example, many chemists who have acquired a deep understanding of the mechanism of branching-chain reactions in closed vessels are completely uninformed about the importance of such processes in flames or detonation waves. This is a severe limitation because the essential feature of all combustion phenomena is that they arise as a result of the interplay of physical and chemical processes and a complete understanding can result only if aspects of mechanical engineering and fluid mechanics are taken into account. The aim of this text is to provide the basic principles which form the background to all combustion phenomena. It is based on a course given to postgraduate students in chemistry at the University of Essex and it is the author's hope that it can be read by final-year undergraduates and research personnel in a wide range of disciplines. The major problem for the author has been that of selection. Because the book is intended to be short, many topics of interest have been omitted and, since decisions as to content have been entirely arbitrary, many readers will disagree with the choice. The author has tried to adhere to certain principles in making the selection. Combustion is an old technology, which at present provides about 90% of our worldwide energy support. Combustion research in the past used fluid mechanics with global heat release by chemical reactions described with thermodynamics, assuming infinitely fast reactions. This approach was useful for stationary combustion processes, but it is not sufficient for transient processes like ignition and quenching or for pollutant formation. Yet pollutant formation during combustion of fossil fuels is a central topic and will continue to be so in future. This book provides a detailed and rigorous treatment of the coupling of chemical reactions and fluid flow. Also, combustion-specific topics of chemistry and fluid mechanics are considered, and tools described for the simulation of combustion processes. Superseding Gardiner's "Combustion Chemistry", this is an updated, comprehensive coverage of those aspects of combustion chemistry relevant to gas-phase combustion of hydrocarbons. The book includes an extended discussion of air pollutant chemistry and aspects of combustion, and reviews elementary reactions of nitrogen, sulfur and chlorine compounds that are relevant to combustion. Methods of combustion modeling and rate coefficient estimation are presented, as well as access to databases for combustion thermochemistry and modeling. This book provides a rigorous treatment of the coupling of chemical reactions and fluid flow. Combustion-specific topics of chemistry and fluid mechanics are considered and tools described for the simulation of combustion processes. This edition is completely restructured. Mathematical Formulae and derivations as well as the space-consuming reaction mechanisms have been replaced from the text to appendix. A new chapter discusses the impact of combustion processes on the atmosphere, the chapter on auto-ignition is extended to combustion in Otto- and Diesel-engines, and the chapters on heterogeneous combustion and on soot formation are heavily revised. Combustion is an old technology, which at present provides about 90% of our worldwide energy support. Combustion research in the past used fluid mechanics with global heat release by chemical reactions described with thermodynamics, assuming infinitely fast reactions. This approach was useful for stationary combustion processes, but it is not sufficient for transient processes like ignition and quenching or for pollutant formation. Yet pollutant formation during combustion of fossil fuels is a central topic and will continue to be so in future. This book provides a detailed and rigorous treatment of the coupling of chemical reactions and fluid flow. Also, combustion-specific topics of chemistry and fluid mechanics are considered, and tools described for the simulation of combustion processes. For the 2nd edition, the parts dealing with experiments, spray combustion, and soot were thoroughly revised. viii and approaches could be adapted to other coal conversion and combustion problems, we have not considered combustion or gasification in fluidized or fixed beds or in situ processes. In addition, we have not considered other fossil-fuel combustion problems associated with oil shale, tar sands, etc., even though many aspects of pulverized-coal combustion would relate to these problems. For the case of pulverized-coal models, we have attempted to provide a detailed description of the model foundations. Parts I and II of this book emphasize general principles for describing reacting, turbulent or laminar, multiphase systems. General conservation equations are developed and summarized. The basis for computing thermochemical equilibrium in complex, heterogeneous mixtures is presented, together with techniques for rapid computation and reference to required input data. Rate processes are then discussed, including pertinent aspects of turbulence, chemical kinetics, radiative heat transfer, and gas-particle convective-diffusive interactions. Much of Part II deals with parameters and coefficients for describing these complex rate processes. This part of the book provides recommended values of coefficients and parameters for treating complex reacting flows. Parts I and II may well be suitable for use in an advanced course in reacting flows, and have been written partly with that in mind. Part III deals with more specific aspects of pulverized-coal characteristics and rate processes. Following a general description of coal structure and constitution, coal pyrolysis and char oxidation processes are considered. Detailed study of the rates and mechanisms of combustion reactions has not been in the mainstream of combustion research until the recent recognition that further progress in optimizing burner performance and reducing pollutant emission can only be done with fundamental understanding of combustion chemistry. This has become apparent at a time when our understanding of the chemistry, at least of small-molecule combustion, and our ability to model combustion processes on large computers have developed to the point that real confidence can be placed in the results. This book is an introduction for outsiders or beginners as well as a reference work for people already active in the field. Because the spectrum of combustion scientists ranges from chemists with little computing experience to engineers who have had only one college chemistry course, everything needed to bring all kinds of beginners up to the level of current practice in detailed combustion modeling is included. It was a temptation to include critical discussions of modeling results and computer programs that would enable outsiders to start quickly into problem solving. We elected not to do either, because we feel that the former are better put into the primary research literature and that people who are going to do combustion modeling should either write their own programs or collaborate with experts. The only exception to this is in the thermochemical area, where programs have been included to do routine fitting operations. For reference purposes there are tables of thermochemical, transport-property, and rate coefficient data. Fundamentals of Combustion Processes is designed as a textbook for an upper-division undergraduate and graduate level combustion course in mechanical engineering. The authors focus on the fundamental theory of combustion and provide a simplified discussion of basic combustion parameters and processes such as thermodynamics, chemical kinetics, ignition, diffusion and pre-mixed flames. The text includes exploration of applications, example exercises, suggested homework problems and videos of laboratory demonstrations Combustion has played a central role in the development of our civilization which it maintains today as its predominant source of energy. The aim of this book is to provide an understanding of both fundamental and applied aspects of low-temperature combustion chemistry and autoignition. The topic is rooted in classical observational science and has grown, through an increasing understanding of the linkage of the phenomenology to coupled chemical reactions, to quite profound advances in the chemical kinetics of both complex and elementary reactions. The driving force has been both the intrinsic interest of an old and intriguing phenomenon and the centrality of its applications to our economic prosperity. The volume provides a coherent view of the subject while, at the same time, each chapter is self-contained. Combustion, the process of burning, is defined as a chemical reaction between a combustible reactant (the fuel) and an oxidizing agent (such as air) in order to produce heat and in most cases light while new chemical species (e.g., flue gas components) are formed. This book covers a gap on the market by providing a concise introduction to combustion. Most of the other books currently available are targeted towards the experienced users and contain too many details and/or contain knowledge at a fairly high level. This book provides a brief and clear overview of the combustion basics, suitable for beginners and then focuses on practical aspects, rather than theory, illustrated by a number of industrial applications as examples. The content is aimed to provide a general understanding of the various concepts, techniques and equipment for students at all level as well as practitioners with little or no prior experience in the field. The authors are all international experts in the field of combustion technology and adopt here a clear didactic style with many practical examples to cover the most common solid, liquid and gaseous fuels. The associated environmental impacts are also discussed so that readers can develop an understanding of the major issues and the options available for more sustainable combustion processes. With a foreword by Katharina Kohse-Höinghaus The scientific and economic importance of the high-temperature reactions of hydrocarbons in both the presence and absence of oxygen cannot be overemphasized. A vast chemical industry exists based on feedstocks produced by the controlled pyrolysis of hydrocarbons, while uncontrolled combustion in air is still among the most important sources of heat and mechanical energy. The detonation and explosion of hydrocarbon-oxidant mixtures can however, be a highly dangerous phenomenon which destroys lives and equipment. In order that control can be exerted over combustion processes, a complete description of hydrocarbon oxidation and pyrolysis is required. A major contribution to this is an understanding of the unstable intermediates involved and their reactions. The aim of this book is to review our knowledge of the chemistry of hydrocarbon combustion and to consider the data which are available for relevant reactions. Chapter 1 describes early studies in which the apparent complexity of the chemistry was established and the type of information required for a better understanding was defined. Experimental studies of the overall process which were carried out with the aim of establishing the sequence of stable chemical intermediates and some of the unstable species are described in Chapter 2. The limited nature of the information thus obtained showed that independent studies of individual reactions involving the unstable species were required. In Chapter 3 investigations specifically aimed at the determination of the kinetics of elementary reactions are discussed. Professionals working in the field of combustion may well find many points of interest, highlighted by the book's logical and global approach to phenomena, which considers mechanical, thermal and chemical aspects simultaneously. The book prioritises an understanding of the physical and chemical aspects of the phenomena, and lays particular emphasis on experimental analyses and modern numerical simulations, and on the way in which these phenomena are translated into equations.Contents: Introduction: Discovering combustion and flames. 1. Combustion thermodynamics. 2. Chemical kinetics applied to combustion. 3. Mass and energy transport by convection and diffusion. 4. Self-ignitions in closed systems. 5. Laminar flames and deflagrations. 6. Turbulent flames and deflagrations. 7. Detonation and supersonic combustion. 8. Flame ignition. 9. Combustion of liquids and sprays. 10. Pollutant emissions in combustion reactions. Index. As the demands for cleaner, more efficient, reduced and zero carbon emitting transportation increase, the traditional focus of Combustion Chemistry research is stretching and adapting to help provide solutions to these contemporary issues. Combustion Chemistry and the Carbon Neutral Future: What will the Next 25 Years of Research Require? presents a guide to current research in the field and an exploration of possible future steps as we move towards cleaner, greener and reduced carbon combustion chemistry. Beginning with a discussion of engine emissions and soot, the book goes on to discuss a range of alternative fuels, including hydrogen, ammonia, small alcohols and other bio-oxygenates, natural gas, syngas and synthesized hydrocarbon fuels. Methods for predicting and improving efficiency and sustainability, such as low temperature and catalytic combustion, chemical looping, supercritical fluid combustion, and diagnostic monitoring even at high pressure, are then explored. Some novel aspects of biomass derived aviation fuels and combustion synthesis are also covered. Combining the knowledge and experience of an interdisciplinary team of experts in the field, Combustion Chemistry and the Carbon Neutral Future: What will the Next 25 Years of Research Require? is an insightful guide to current and future focus areas for combustion chemistry researchers in line with the transition to greener, cleaner technologies. Provides insight on current developments in combustion chemistry as a tool for supporting a reduced-carbon future Reviews modeling and diagnostic tools, in addition to key approaches and alternative fuels Includes projections for the future from leaders in the field, pointing current and prospective researchers to potentially fruitful areas for exploration Throughout its previous four editions, Combustion has made a very complex subject both enjoyable and understandable to its student readers and a pleasure for instructors to teach. With its clearly articulated physical and chemical processes of flame combustion and smooth, logical transitions to engineering applications, this new edition continues that tradition. Greatly expanded end-of-chapter problem sets and new areas of combustion engineering applications make it even easier for students to grasp the significance of combustion to a wide range of engineering practice, from transportation to energy generation to environmental impacts. Combustion engineering is the study of rapid energy and mass transfer usually through the common physical phenomena of flame oxidation. It covers the physics and chemistry of this process and the engineering applications—including power generation in internal combustion automobile engines and gas turbine engines. Renewed concerns about energy efficiency and fuel costs, along with continued concerns over toxic and particulate emissions, make this a crucial area of engineering. New chapter on new combustion concepts and technologies, including discussion on nanotechnology as related to combustion, as well as microgravity combustion, microcombustion, and catalytic combustion—all interrelated and discussed by considering scaling issues (e.g., length and time scales) New information on sensitivity analysis of reaction mechanisms and generation and application of reduced mechanisms Expanded coverage of turbulent reactive flows to better illustrate real-world applications Important new sections on stabilization of diffusion flames—for the first time, the concept of triple flames will be introduced and discussed in the context of diffusion flame stabilization Non-uniform combustion, as encountered in diesel and gas turbine engines, furnaces, and boilers, is responsible for the conversion of fossil fuel to energy and also for the corresponding formation of pollutants. In spite of great research efforts in the past, the mechanism of non-uniform combustion has remained less explored than that of other combustion types, since it consists of many, mostly transient processes which influence each other. In view of this background, a group research project, "Exploration of Combustion Mechanism", was established to explore the mechanism of combustion, especially that of diffusive combustion, and also to find efficient ways to control the combustion process for better utilization of fuel and the reduction of pollutant emission. The group research was started, after preparatory activity of 2 years, in April 1988, for a period of 3 years, as a project with a Grant-in-Aid for Scientific Research of Priority Area subsidized by the Ministry of Education, Science and Culture of Japan. The entire group of 43 members was set up as an organizing committee of 13 members, and five research groups, consisting of 36 members. The research groups were: (1) Steady combustion, (2) Unsteady spray combustion, (3) Control of combustion, (4) Chemistry of combustion, and (5) Effects of fuels. At the beginning of the project it was agreed that we should pursue the mechanism of combustion from a scientific viewpoint, namely, the target of the project was to obtain the fundamentals, or "know why", rather than "know how" of combustion. On March 30, 1981, a symposium entitled "Chemistry of Engine Combustion Deposits" was held at the 181st American Chemical Society National Meeting in Atlanta, Georgia, under the sponsorship of the Petroleum Division. This book is an out growth of that symposium, including papers from all of the At 1 anta presentors, as we 11 as from others who were i nvi ted to contribute. Research on engine deposits has not been as "glamorous" as in the rel ated fossil fuel areas of petrol eum, coal, or oil shale, and publications in the field have been largely confined to combustion and automotive engineering journals. One objec tive of this book is to bring a large body of work on the chemistry of deposits into more general accessibility. We hope to make people more familiar with what deposits are, with what problems they cause, and with what present workers are doing to solve these problems. The creation of the book has involved many people. Patricia M. Vann of Plenum Publishing Corporation gave guidance in planning. We thank Claire Bromley, Ellen Gabriel, and Halina Markowski for the preparation of many of the Exxon contribu tions. Finally, we thank Joseph C. Scanlon for his useful advice and encouragement. Detailed study of the rates and mechanisms of combustion reactions has not been in the mainstream of combustion research until the recent recognition that further progress in optimizing burner performance and reducing pollutant emission can only be done with fundamental understanding of combustion chemistry. This has become apparent at a time when our understanding of the chemistry, at least of small-molecule combustion, and our ability to model combustion processes on large computers have developed to the point that real confidence can be placed in the results. This book is an introduction for outsiders or beginners as well as a reference work for people already active in the field. Because the spectrum of combustion scientists ranges from chemists with little computing experience to engineers who have had only one college chemistry course, everything needed to bring all kinds of beginners up to the level of current practice in detailed combustion modeling is included. It was a temptation to include critical discussions of modeling results and computer programs that would enable outsiders to start quickly into problem solving. We elected not to do either, because we feel that the former are better put into the primary research literature and that people who are going to do combustion modeling should either write their own programs or collaborate with experts. The only exception to this is in the thermochemical area, where programs have been included to do routine fitting operations. For reference purposes there are tables of thermochemical, transport-property, and rate coefficient data. The preservation of the environment is of increasing concern at all scales, from individual countries through continents to the entire planet. Combustion is known to contribute substantially to damage to the atmosphere and therefore this book reviews current knowledge of the mechanisms by which the main pollutants are formed in combustion systems. In most situations, pollutants are present as trace components and their formation and removal is strongly conditioned by the chemical reactions initiated by fuel consumption. Specific papers therefore define precisely the general properties of combustion chemistry for gaseous, liquid and solid fuels. A substantial part of the work also concerns the impact on atmospheric chemistry of the main combustion pollutants: NOx, aromatics, soot, VOCs, sulfur and chlorinated compounds. It is this combination of combustion and atmospheric chemistry that gives the book its unique character. Chemical Physics of Pyrolysis, Combustion & Oxidation Combustion is very much an interdisciplinary topic, drawing together elements of chemistry, fluid mechanics and heat transfer. It is an ingredient in many undergraduate degree programmes, ranging from a pivotal role in fuel science through to a component part of courses in chemical, process and building services engineering. For many students in those disciplines where combustion in heating plant is an important part of their studies, there are often problems in coming to grips with the basic principles underlying the combustion of hydrocarbon fuels. In particular, the concepts of chemical and related thermodynamic changes can prove difficult to assimilate. The scientific literature dealing with combustion tends to be rather polarised, with a wealth of literature aimed at the specialist reader, but at a basic level the fundamentals of this important process are often treated rather tersely in textbooks on thermodynamics. The objective of this book is to provide an introduction to the basic principles of the combustion of hydrocarbon fuels in heating plant for buildings and industrial processes. In those chapters where practice in problem solving can make a positive contribution to understanding, some numerical problems have been included. Acknowledging the ever-widening use of computers in technical education, a number of algorithms which can be easily coded up for solving numerical problems have been incorporated in the text. These can prove particularly useful in, for example, the calculation of certain fluid properties, either for use in hand calculation or for incorporation into larger programs. Most of the material covered in this book deals with the fundamentals of chemistry and physics of key processes and fundamental mechanisms for various combustion and combustion related phenomena in gaseous combustible mixture. It provides the reader with basic knowledge of burning processes and mechanisms of reaction wave propagation. The combustion of a gas mixture (flame, explosion, detonation) is necessarily accompanied by motion of the gas. The process of combustion is therefore not only a chemical phenomenon but also one of gas dynamics. The material selection focuses on the gas phase and with premixed gas combustion. Premixed gas combustion is of practical importance in engines, modern gas turbine and explosions, where the fuel and air are essentially premixed, and combustion occurs by the propagation of a front separating unburned mixture from fully burned mixture. Since premixed combustion is the most fundamental and potential for practical applications, the emphasis in the present work is be placed on regimes of premixed combustion. This text is intended for graduate students of different specialties, including physics, chemistry, mechanical engineering, computer science, mathematics and astrophysics. This unique book investigates the synthesis, kinetics, and thermal decomposition properties and processing of energy-producing materials used in propellants, explosives, pyrotechnic, and gas-generating compositions. Thermal Decomposition and Combustion of Explosives and Propellants provides several mechanisms and stages for the thermal decomposition and combustion reactions of most flammable compounds and their mixtures, such asaliphatic and aromatic nitrocompounds, nitramines, nitroesters, organic azides, furazanes, tetrazols, difluoroamines, polynitrous heterocycles, and onium salts. The authors examine the classic problem of the dependence of explosive activity on molecular structure, using applications to predict the stability, compatibility, and the stabilization of explosives and propellant components. They also offer experimental results examining factors such as subsurface decomposition, evaporation, and dispersion of materials, which can be used to control combustion of condensed systems. Providing several approaches to stability, safety, and controlled combustion of flammable substances, Thermal Decomposition and Combustion of Explosives and Propellants is a multi-dimensional resource for graduate students, researchers and professionals interested in chemical kinetics, the combustion and synthesis of high-energy materials, criminal forensics, and the field of explosives, powders, and solid rocket propellants. The utilization of mathematical models to numerically describe the performance of internal combustion engines is of great significance in the development of new and improved engines. Today, such simulation models can already be viewed as standard tools, and their importance is likely to increase further as available com puter power is expected to increase and the predictive quality of the models is constantly enhanced. This book describes and discusses the most widely used mathematical models for in-cylinder spray and combustion processes, which are the most important subprocesses affecting engine fuel consumption and pollutant emissions. The relevant thermodynamic, fluid dynamic and chemical principles are summarized, and then the application of these principles to the in-cylinder processes is ex plained. Different modeling approaches for the each subprocesses are compared and discussed with respect to the governing model assumptions and simplifica tions. Conclusions are drawn as to which model approach is appropriate for a specific type of problem in the development process of an engine. Hence, this book may serve both as a graduate level textbook for combustion engineering stu dents and as a reference for professionals employed in the field of combustion en gine modeling. The research necessary for this book was carried out during my employment as a postdoctoral scientist at the Institute of Technical Combustion (ITV) at the Uni versity of Hannover, Germany and at the Engine Research Center (ERC) at the University of Wisconsin-Madison, USA. This volume contains invited lectures and contributed papers presented at the NATO Advanced Research Workshop on Mathematical Modeling in Combustion and related topics, held in. Lyon (France), April 27 - 30, 1987. This conference was planned to fit in with the two-month visit of Professor G.S.S. Ludford to the Ecole Centrale de Lyon. He kindly agreed to chair the Scientific and Organizing Committee and actively helped to initiate the meeting. His death in December 1986 is an enormous loss to the scientific community in general, and in particular, to the people involved in the present enterprise. The subject of mathematical modeling in combustion is too large for a single conference, and the selection of topics re flects both areas of recent research activity and areas of in terest to Professor G.S.S. Ludford, to whose memory the Advanced Workshop and this present volume are dedicated. The meeting was divided into seven specialized sessions detonation theory, mathematical analysis, numerical treatment of combustion problems, flame theory, experimental and industrial aspects, complex chemistry, and turbulent combustion. It brought together researchers and engineers from University and Industry (see below the closing remarks of the workshop by Prof. N. Peters). The articles in this volume have been judged and accepted on their scientific quality, and language corrections may have been sacrificed in order to allow quick dissemination of knowledge to prevail. This book contains a collection of papers prepared by leading experts on selected areas of particular importance to researchers in combustion science. The editors have gathered writings on fundamental physical and chemical aspects of combustion, including combustion chemistry, soot formation, and condensed phase and turbulent combustion intended to be a source of current understanding on the topics covered. The materials were originally presented as part of a Colloquium on Combustion held in honor of Professor Irvin Glassman. The Institute for Computer Applications in Science and Engineer ing (ICASE) and NASA Langley Research Center (LaRC) brought together on October 2-4, 1989 experts in the various areas of com bustion with a view to expose them to some combustion problems of technological interest to LaRC and possibly foster interaction with the academic community in these research areas. The top ics chosen for this purpose were flame structure, flame stability, flame holding/extinction, chemical kinetics, turbulence-kinetics in teraction, transition to detonation, and reacting free shear layers. The lead paper set the stage by discussing the status and issues of supersonic combustion relevant to scramjet engine. Then the ex perts were called upon i) to review the current status of knowledge in the aforementioned ;:I. reas, ii) to focus on how this knowledge can be extended and applied to high-speed combustion, and iii) to suggest future directions of research in these areas. Each topic was then dealt with in a position paper followed by formal discussion papers and a general discussion involving the participants. The position papers discussed the state-of-the-art with an emphasis on key issues that needed to be resolved in the near future. The discussion papers crit ically examined these issues and filled in any lacunae therein. The edited versions of the general discussions in the form of questions from the audience and answers from the speakers are included wher ever possible to give the reader the flavor of the lively interactions that took place. Introduces advanced mathematical tools for the modeling, simulation, and analysis of chemical non-equilibrium phenomena in combustion and flows, following a detailed explanation of the basics of thermodynamics and chemical kinetics of reactive mixtures. Researchers, practitioners, lecturers, and graduate students will find this work valuable. An introduction for postgraduate and undergraduate students to the chemical and physical principles of flame and combustion phenomena. This book should be of interest to undergraduate/postgraduate chemists; chemical engineers; undergraduate/postgraduate mechanical engineers and environmental scientists; and industrial combustion technologists. These two volumes represent the culmination of the Special Year `84-'85 in Reacting Flows held at Cornell University. As the proceedings of the 1985 AMS/SIAM Summer Seminar in Applied Mathematics, the volumes focus on both mathematical and computational questions in combustion and chemical reactors. They are addressed to researchers and graduate students in the theory of reacting flows. Together they provide a sound basis and many incentives for future research, especially in computational aspects of reacting flows. Although the theory of reacting flows has developed rapidly, researchers in the two subareas of combustion and chemical reactors have not communicated. The main goal of this seminar was to synthesize the mathematical theory and bring it to the interface with large-scale computing. All of the papers have high research value, but the first five introductory lectures should be especially noted.