Gas-Phase Combustion Chemistry

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Preface

This book differs from its out of print 1984 predecessor¹ primarily by lacking theoretical chapters on combustion modeling and elementary reaction rate coefficients. While noteworthy advances in these subjects have been made since 1984, it was decided to mention theory in this book only where appropriate in chapters describing combustion chemistry itself. Otherwise, space limitation would have forced us to discuss only new developments in theoretical areas, thereby abandoning our goal of keeping this book readable by newcomers to the field of combustion modeling. Contemporary modeling and rate coefficient theory as applied to combustion deserve a book of their own.

A second omission is a chapter devoted to reviewing the elementary reactions that contribute to the combustion chemistry of hydrogen, carbon monoxide, and hydrocarbon or alternate fuels. Readers looking for guidance to the current knowledge we have in this area will find a broad outline and extensive references to the review and archival literature in Chapter 1, where the essential features of combustion chemistry modeling are surveyed.

The heart of this book is its chapters on the combustion chemistry of nitrogen, sulfur, and chlorine. Nitrogen and sulfur draw interest mostly because their oxides are the primary pollutants formed in combustion, chlorine because it is the prototype flame inhibitor and because incineration of toxic waste faces the challenge of reducing the concentrations of chlorine-containing organic compounds in waste streams to extremely low levels. It will be clear to all readers that while many molecular-level details have been discovered about the high-temperature chemistry of these elements, our ability to describe in combustion simulations what has been measured in combustion experiments is still limited by the incompleteness of our chemical understanding.

Like most basic combustion research, this book deals with what happens in the gas phase. Condensed phase chemistry relevant to explosives and propellants is not specifically addressed, although many elementary reactions relevant to that chemistry also play roles in gas-phase combustion. Two-phase combustion reactions, including formation and oxidation of soot, combustion of coal char and formation of inorganic ash, and the influence of chamber walls on nearby flames are likewise not described. These are certainly important chemical processes, but, aside from soot particle nucleation, modeling of two-phase combustion has so far been mostly limited to empirical descriptions that do not attempt to capture chemical detail in a fundamental way. On the other hand, there are some high temperature gas-phase reactions—such as chemiluminescence, ion formation, and reactions of metals—for which we do have molecular-level knowledge but which have remained at the periphery of combustion science. Readers interested in topics like these can readily gain entrance to the relatively limited literature¹ on them;

¹ *Combustion Chemistry*, W.C. Gardiner, Ed., Springer-Verlag, New York 1984.

¹ Beginning with the biennial International Combustion Symposium volumes published by the Combustion Institute in Pittsburgh.

thoughtful reading of Chapter 1 will provide all the background needed to place such special interests in context with the mainstream of combustion chemistry modeling.

Much of the content found here can be supplemented with resources on the Internet and the World Wide Web. We have tried to include URLs for all of the relevant sites that we know about, but some have surely been overlooked and many new ones will be established before this book becomes obsolete. Despite the limited lifetimes and uncertain reliability of Internet resources, creators and users of combustion chemistry knowledge generally have such Internet-friendly personalities that we expect to see essentially all of the combustion chemistry database and most of the computational resources one needs to utilize it on-line before this book is out of print.

Austin, Texas

William C. Gardiner, Jr.

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