Kenneth K. Kuo · Ragini Acharya

Applications of Turbulent and Multiphase Combustion

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Ken Kuo would like to dedicate this book to his wife, Olivia (Jeon-lin), and their daughters, Phyllis and Angela, for their love, understanding, patience, and support, and to his mother, Mrs. Wen-Chen Kuo, for her love and encouragement.

Ragini Acharya would like to dedicate this book to her parents, Meenakshi and Krishnama Acharya, for their love, patience, and support and for having endless faith in her.

PREFACE

There is an ever-increasing need to understand turbulent and multiphase combustion due to their broad application in energy, environment, propulsion, transportation, industrial safety, and nanotechnology. More engineers and scientists with skills in these areas are needed to solve many multifaceted problems. Turbulence itself is one of the most complex problems the scientific community faces. Its complexity increases with chemical reactions and even more in the presence of multiphase flows.

A number of useful books have been published recently in the areas of theory of turbulence, multiphase fluid dynamics, turbulent combustion, and combustion of propellants. These include *Theoretical and Numerical Combustion* by Poinsot and Veynante; *Turbulent Flows* by Pope; *Introduction to Turbulent Flow* by Mathieu and Scott; *Turbulent Combustion* by Peters; *Multiphase Flow Dynamics* by Kolev; *Combustion Physics* by Law; *Fluid Dynamics and Transport of Droplet and Sprays* by Sirignano; *Compressible, Turbulence, and High-Speed Flow* by Gatski and Bonnet; *Combustion* by Glassman and Yetter, among others.

Kenneth Kuo, the first author of this book, previously published *Principles of Combustion*. The second edition, published in 2005, contains comprehensive material on laminar flames, chemical thermodynamics, reaction kinetics, and transport properties for multicomponent mixtures. As the research in laminar flames was overwhelming, he decided to develop two separate books dedicated entirely to turbulent and multiphase combustion.

Turbulence, turbulent combustion, and multiphase reacting flows have been major research topics for many decades, and research in these areas is expected to continue at even a greater pace. Usually the research has focused on experimental studies with phenomenological approaches, resulting in the development of empirical correlations. Theoretical approaches have achieved some degree of success. However, in the past 20 years, advances in computational capability have enabled significant progress to be made toward comprehensive theoretical modeling and numerical simulation. Experimental diagnostics, especially nonintrusive laser-based measurement techniques, have been developed and used to obtain accurate data, which have been used for model validation. There is a greater synergy between the experimental and theoretical/numerical approaches. Due to these ongoing developments and advancements, theoretical modeling and numerical simulation hold great potential for future solutions of problems. In these two new books, we have attempted to integrate the fundamental theories of turbulence, combustion, and multiphase phenomena as well as experimental techniques, so that readers can acquire a firm background in both contemporary and classical approaches. The first book volume is called *Fundamentals of Turbulent and Multiphase Combustion*; the second is called *Applications of Turbulent and Multiphase Combustion.* The first volume can serve as a graduate-level textbook that covers the area of turbulent combustion and multiphase reacting flows as well as material that builds on these fundamentals. This volume also can be useful for research purpose. It is oriented toward the theories of combustion, turbulence, multiphase flows, and turbulent jets. Whenever appropriate, experimental setups and results are provided. The first volume addresses eight basic topical areas in combustion and multiphase flows, including laminar premixed and nonpremixed flames; theory of turbulence; turbulent premixed and nonpremixed flames; background of multiphase flows; and spray atomization and combustion. A deep understanding of these topics is necessary for researchers in the field of combustion.

The six chapters in the second volume build on the ground covered in the first volume. Its chapters include: solid propellant combustion, thermal decomposition and combustion of nitramines burning behavior of homogeneous solid propellants, chemically reacting boundary-layer flows, ignition and combustion of combustion of single energetic solid particles, and combustion of solid particles in multiphase flows. The major reason for including solid-propellant combustion here is to provide concepts for condensed-phase combustion modeling as an example. Nitramines are explosive or propellant ingredients; their decomposition and reaction mechanisms are also good examples for combustion behavior of condensed-phase materials. Chapters in Volume 2 focus on the application aspect of fundamental concepts and can form the framework for an advanced graduate-level course in combustion of condensed-phase materials. However, the selection of materials for instruction depends extirely on the interests of instructors and students. Although several chapters address solid propellant combustion, this volume is not a textbook for solid propellant combustion; many topics in this area are not included due to space limitations.

VOLUME 1, FUNDAMENTALS OF TURBULENT AND MULTIPHASE COMBUSTION

Chapter 1 introduces and stresses the importance of combustion and multiphase flows in research. It also provides a succinct review of major conservation equations. Appendix A provides the vector and tensor operations frequently used in the formulation and manipulation of these equations.

Chapter 2 covers the basic structure of laminar premixed flames, conservation equations, various models for diffusion velocities in a multicomponent gas system with increasing complexities, laminar flame thickness, asymptotic analyses, and flame speeds. Effect of flame stretch on laminar flame speed, Karlovitz number, and Markstein lengths are also discussed in detail along with soot formation in laminar premixed flames.

Chapter 3 discusses the basic structure of laminar nonpremixed flames and provides detailed descriptions of mixture fraction definition, balance equations for mixture fraction, temperature-mixture fraction relationship, and examples, since mixture fraction is a very important parameter in the study of nonpremixed flames. The chapter also discusses laminar flamelet structure and equations, critical scalar dissipation rate, steady-state combustion, and examples of laminar diffusion flames with equations and solutions. Since pollution, specifically soot formation, has become a major topic of interest, it is also covered in this chapter with respect to laminar diffusion flames. Appendix D provides a detailed soot formation mechanism and rate constants that was proposed by Wang and Frenklach.

Chapter 4 is devoted entirely to turbulent flows. It covers the fundamental understanding of turbulence from a statistical point of view; homogeneous and/or isotropic turbulence, averaging procedures, statistical moments, and correlation functions; Kolmogorov hypotheses; turbulent scales; filtering and large-eddy simulation (LES) concepts along with various subgrid scale models; and basic definitions to prepare readers for the probability density function (pdf) approach in later chapters. This chapter also includes the governing equations for compressible flows. A short introduction of the direct numerical simulation (DNS) approach is also provided at the end of the chapter.

Chapters 5 and 6 focus on the turbulent premixed and nonpremixed flames, respectively. Chapter 5 consists of physical interpretation; studies for turbulent flame-speed correlation development; Borghi diagram and physical interpretation of various regimes; eddy breakup models; measurements in premixed turbulent flames; flame-turbulence interaction (effects of turbulence on flame as well as effect of flame on turbulence); turbulence combustion modeling approaches; Bray-Moss-Libby model (gradient and counter-gradient transport); level set approach and G-equation for flame surfaces; and the pdf approach and closure of chemical reaction source term. In Chapter 6, the discussion focuses on major problems in nonpremixed turbulent combustion; turbulent Damköhler number and Reynolds number; scales in nonpremixed turbulent flames; regime diagrams; target flames; turbulence-chemistry interaction; pdf approach; flamelet models; flame-vortex interaction; flame instability; partially premixed flames; and edge flames.

The fundamentals of multiphase flows are covered in Chapter 7, which has sections on classification of multiphase flows; homogeneous versus multiphase mixtures; averaging methods; local instant formulation; Eulerian-Eulerian modeling; Eulerian-Lagrangian modeling; interface transport (tracking and capturing) methods (volume of fluid, surface fitted method, markers on interface); and discrete particle methods. This chapter also provides many contemporary approaches for modeling two-phase flows.

Spray combustion is an extremely important topic for combustion, and Chapter 8 provides a comprehensive account of various modeling approaches to spray combustion associated with single drop behavior, drop breakup mechanisms, jet breakup models, group combustion models, droplet-droplet collisions, and dense sprays. Experimental approaches and results are also presented in this chapter.

VOLUME 2, APPLICATIONS OF TURBULENT AND MULTIPHASE COMBUSTION

Chapter 1 provides a background in solid propellants and their combustion behavior, including desirable characteristics; oxygen balance; homogeneous and heterogeneous propellants; fuel binders, oxidizer ingredients, curing and cross-linking agents, and aging; hazard classifications; material characterization of solid propellants; and gun performance parameters including thrust, specific impulse, and stable/unstable burning behavior.

Chapter 2 focuses on nitramine decomposition and combustion; phase transformation; and three different approaches for thermal decomposition of royal demolition explosive (RDX) as well as gas-phase reactions. This chapter also describes a modeling approach for RDX combustion.

Chapter 3 covers the burning behavior of homogeneous (e.g., double-base) propellants, describing both the experimental and modeling approaches to study and predict the burning rate and temperature sensitivities of common solid propellants. The transient burning characteristics of a typical homogeneous propellant is also presented in detail, including the Zel'dovich map technique and the Novozhilov stability parameters.

Chapter 4 covers reacting turbulent boundary-layer flows, a topic of research for the last six decades. The chapter discusses the modeling approaches from 1940s to the current date. Graphite nozzle erosion process by high-temperature combustion product gases through heterogeneous chemical reactions is covered in detail. Turbulent wall fires are also covered.

Chapter 5 contains the ignition and combustion studies of single energetic particles (such as micron-size boron and aluminum particles) including multistage combustion models for cases with and without the presence of oxide layers, kinetic mechanisms, criterion for diffusion-controlled combustion versus, kinetic controlled combustion, effect of oxidizers (such as oxygen- and fluorine-containing species), combustion of nano-size energetic particles, and their strong dependency on kinetic rates.

Chapter 6 addresses the two-phase reacting flow simulation and focuses on granular bed combustion with different solution techniques for the governing equations. It also includes experimental validation of the calculated results.

We would like to acknowledge the contributions of many of our combustion and turbulence colleagues for reviewing and providing a critical assessment

of multiple chapters of these volumes includes Professor Forman A. Williams of the University of California-San Diego; Professor Stephen B. Pope, Cornell University; Dr. Richard Behrens, Jr. of Sandia National Laboratory; Dr. William R. Anderson of the U.S. Army Research Laboratory; Professor Luigi T. DeLuca of Politecnico di Milano, Italy; and Professors James G. Brasseur, Daniel C. Haworth, and Michael M. Micci of Pennsylvania State University. They spent their valuable time reading chapters and helped us to improve the material covered in Volume 1 and Volume 2. We also want to thank Professor Michael Frenklach of University of California-Berkeley for providing us the detailed information on soot formation kinetics used in Appendix D of Volume 1. We also like to thank Professor William A. Sirignano of University of California-Irvine for his valuable input on evaporation and combustion of droplet arrays. Professor Norbert Peters of the Institut für Technische Mechanik of Aachen, Germany, was very geneous to provide his book draft to Kenneth Kuo while he was visiting the Pennsylvania State University. His notes were very helpful in explaining turbulent combustion topics.

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