Cambridge University Press & Assessment
978-1-107-06745-5 — Combustion Thermodynamics and Dynamics
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COMBUSTION THERMODYNAMICS AND DYNAMICS

Combustion Thermodynamics and Dynamics builds on a foundation of thermal science, chemistry, and applied mathematics that will be familiar to most undergraduate aerospace, mechanical, and chemical engineers to give a first-year graduate level exposition of the thermodynamics, physical chemistry, and dynamics of advection-reaction-diffusion. Special effort is made to link notions of time-independent classical thermodynamics with time-dependent reactive fluid dynamics. In particular, concepts of classical thermochemical equilibrium and stability are discussed in the context of modern nonlinear dynamical systems theory. The first half emphasizes time-dependent spatially homogeneous reaction, while the second half considers effects of spatially inhomogeneous advection and diffusion on the reaction dynamics. Attention is focused on systems with realistic detailed chemical kinetics as well as simplified kinetics. Many mathematical details are presented, and several quantitative examples given. Topics include foundations of thermochemistry, reduced kinetics, reactive Navier-Stokes equations, reaction-diffusion systems, laminar flame, oscillatory combustion, and detonation.

Joseph M. Powers is a professor in the Department of Aerospace and Mechanical Engineering at the University of Notre Dame. His research uses computational science to consider the dynamics of high-speed reactive fluids, especially as it applies to verification and validation of complex multiscale systems. He has held positions at the NASA Lewis Research Center, the Air Force Research Laboratory, the Los Alamos National Laboratory, and the Chinese Academy of Sciences. He is editor-in-chief of the AIAA's *Journal of Propulsion and Power*, an Associate Fellow of AIAA, and a member of APS, ASME, the Combustion Institute, and SIAM. He is the recipient of numerous teaching awards.

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www.cambridge.org
Information on this title: www.cambridge.org/9781107067455

First published 2016

A catalogue record for this publication is available from the British Library

Library of Congress Cataloging-in-Publication data
Names: Powers, Joseph, 1961– author.
Title: Combustion thermodynamics and dynamics / Joseph M. Powers.
Description: New York, NY : Cambridge University Press, [2016] | Includes bibliographical references and index.
Identifiers: LCCN 2015047025 | ISBN 9781107067455 (hardback : alk. paper)
Subjects: LCSH: Combustion – Mathematical models. | Thermodynamics – Mathematics.
Classification: LCC QD516 .P667 2016 | DDC 541/.361 – dc23
LC record available at http://lccn.loc.gov/2015047025

ISBN 978-1-107-06745-5 Hardback

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Preface

This book considers mathematical modeling of combustion, in particular, its time-independent thermodynamics and its relation to time-dependent dynamics. A major goal is to more fully incorporate the methods and language of nonlinear dynamical systems analysis (e.g., equilibria, phase space, sources, sinks, saddles, and limit cycles) into the pedagogy of traditional combustion theory. A second major goal is to consider problems that show how the mechanisms of advection, reaction, and diffusion influence the multiscale features of combustion systems' evolution in space and time. The largest fraction of the book is an exposition of some standard material of combustion science. This is accompanied by original work of the author that has been a part of his graduate course lectures and some of the specialized work of the author, his students, and colleagues on relevant topics, especially model reduction, thermodynamics of irreversible processes, identification of length and time scales of one-dimensional unsteady systems, multiscale dynamics, and detonation theory, which has been adapted from studies that have appeared in the archival combustion literature.

The focus is on deterministic continuum models of gas phase combustion, solution methods, detailed development of analytical results, and physical interpretations. As computational methods and hardware expand in their capability, it is useful to take stock of what deterministic modeling can offer, and some of our examples are to this end. Indeed, practical combustion problems abound that do not yield to deterministic continuum methods. Nevertheless, the rapid insights for causality they afford will long render such models as playing a leading role in combustion science.

This book arose from lecture notes for AME 60636, Fundamentals of Combustion, a graduate course taught since 1994 in the Department of Aerospace and Mechanical Engineering of the University of Notre Dame. Many undergraduates with standard preparation in thermodynamics, fluid dynamics, linear algebra, and differential equations have successfully completed the course. The book can guide a semester-long course, although some topics may need to be omitted.

Part I is devoted to time-independent thermodynamics of reactive mixtures and time-dependent systems that are restricted to spatially homogeneous reaction, thus avoiding the significant complications that come with advection and diffusion. Chapter 1 gives a discussion of the reaction dynamics of some simple but realistic time-dependent gas phase chemistry. These examples bring to the fore many of the important topics of the book: posing of combustion problems as nonlinear dynamical systems, identification of equilibria, time stability of equilibria via local linear analysis, phase space analysis, and full nonlinear dynamics. Next, in the spirit of physical chemistry, the thermodynamics of reacting gas mixtures is presented. Chapter 2 considers Dalton's mixture theory. Chapter 3 presents the thermodynamics of reacting mixtures, including equilibrium thermochemistry. Chapter 4 considers the time dynamics of a single reaction, followed by its multistep equivalent in Chapter 5. Special attention is given to the topic of irreversible entropy production and its interplay with combustion dynamics. A small discussion of the large topic of model reduction is given in Chapter 6, focusing mainly on dynamical systems aspects; a brief consideration of the significantly complicating effects of diffusion closes the chapter and serves as a bridge to Part II.

Part II considers various combinations of advection and diffusion within reactive systems. Chapter 7 presents the reactive Navier-Stokes equations with detailed kinetics and multicomponent diffusion. Chapter 8 presents an idealized linear model of advection-reaction-diffusion with a simplicity that allows many features of multiscale dynamics to be exposed. Chapter 9 returns to nonlinear dynamics of systems with reaction and diffusion. Chapter 10 considers the well-studied field of premixed one-dimensional laminar flames in the context of a simple advection-reaction-diffusion model that admits a compact presentation as a dynamical system. Chapter 11 briefly considers systems that do not relax to a stationary equilibrium but rather to a long time limit cycle. We close in Chapter 12 with an extended discussion of one-dimensional detonation theory as it is connected with nonlinear dynamics. Each chapter is concluded with a few exercises appropriate for homework. The problems are either self-contained or may need standard information from a thermodynamics text. Instructors with access to software for detailed chemical kinetics can and should be able to develop problems harnessing these tools that enable consideration of a broader range of mixtures important for engineering applications. Because these software tools rapidly change and rely on specific computing systems, we have included no detailed descriptions.

Quantitative predictions are presented in detail to enable the reader to reproduce most results. Often more significant digits than are justified by experiment are presented to this end. Typically, ideal gases are considered with either modestly sized models of detailed kinetics (e.g., H_2-air, oxygen dissociation, or nitrous oxide formation) or one-step kinetics. The book is more general than a monograph and more focused than a comprehensive text. Largely absent are important topics in combustion well covered in the cited literature: turbulence and spray modeling, multidimensional effects, radiation, experimental validation, and so on. Most of these topics are of sufficient complexity that they do not readily lend themselves to compact analysis as a dynamical system.

Many of the chapters reflect the significant interaction of the author with his students, colleagues, and teachers, with support from the U.S. National Science Foundation, NASA, and the U.S. Department of Energy. The author is grateful to the long years of dedicated, patient scholarship shown by his PhD students in combustion over the years: M. J. Grismer, K. A. Gonthier, S. Singh, A. K. Henrick, A. N. Al-Khateeb, J. D. Mengers, and C. M. Romick. Their work infuses this book, as does that of colleagues S. Paolucci and T. D. Aslam. And it is hoped that the guidance and wisdom of advisers H. Krier and D. S. Stewart, teacher J. D. Buckmaster, colleague P. B. Butler, and dozens of friends in the broader combustion community are reflected in the text.