Turbulent Combustion

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 gas expansion and 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, nonpremixed, 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.

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CAMBRIDGE MONOGRAPHS ON MECHANICS

TURBULENT COMBUSTION

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CAMBRIDGE
UNIVERSITY PRESS

PUBLISHED BY THE PRESS SYNDICATE OF THE UNIVERSITY OF CAMBRIDGE
The Pitt Building, Trumpington Street, Cambridge, United Kingdom

CAMBRIDGE UNIVERSITY PRESS
The Edinburgh Building, Cambridge CB2 2RU, UK
40 West 20th Street, New York, NY 10011-4211, USA
477 Williamstown Road, Port Melbourne, VIC 3207, Australia
Ruiz de Alarcón 13, 28014 Madrid, Spain
Dock House, The Warterfront, Cape Town 8001, South Africa

http://www.cambridge.org

First published 2000
Reprinted 2002, 2004 (with corrections)

Printed in the United Kingdom at the University Press, Cambridge

Typeface Times Roman 10/13 pt. *System* LaTeX 2$_\varepsilon$ [TB]

A catalog record for this book is available from the British Library.

Library of Congress Cataloging in Publication Data

Peters, Norbert.
Turbulent combustion / N. Peters.
p. cm. – (Cambridge monographs on mechanics)
Includes bibliographical references.
ISBN 0-521-66082-3
1. Combustion engineering. 2. Turbulence. I. Title. II. Series.
TJ254.5. .P48 2000
621.402′3 – dc21 99-089451

ISBN 0 521 66082 3 hardback

To Cordula

Contents

Cambridge University Press
0521660823 - Turbulent Combustion
Norbert Peters
Frontmatter
More information

Cambridge University Press
0521660823 - Turbulent Combustion
Norbert Peters
Frontmatter
More information

Preface

Fossil fuels remain the main source of energy for domestic heating, power generation, and transportation. Other energy sources such as solar and wind energy or nuclear energy still account for less than 20% of total energy consumption. Therefore combustion of fossil fuels, being humanity's oldest technology, remains a key technology today and for the foreseeable future. It is well known that combustion not only generates heat, which can be converted into power, but also produces pollutants such as oxides of nitrogen (NO_x), soot, and unburnt hydrocarbons (HC). Ever more stringent regulations are forcing manufacturers of automotives and power plants to reduce pollutant emissions, for the sake of our environment. In addition, unavoidable emissions of CO_2 are believed to contribute to global warming. These emissions will be reduced by improving the efficiency of the combustion process, thereby increasing fuel economy.

In technical processes, combustion nearly always takes place within a turbulent rather than a laminar flow field. The reason for this is twofold: First, turbulence increases the mixing processes and thereby enhances combustion. Second, combustion releases heat and thereby generates flow instability by buoyancy and gas expansion, which then enhances the transition to turbulence.

This book addresses gaseous turbulent flows only. Although two-phase turbulent flows such as fuel sprays are also of much practical interest, they are omitted here, because their fundamentals are even less well understood than those of turbulent combustion. We also restrict ourselves to low Mach number flows, because high speed turbulent combustion is an area of its own, with practical applications in supersonic and hypersonic aviation only.

Technical processes in gaseous turbulent combustion can be subdivided in terms of mixing: premixed, nonpremixed, or partially premixed turbulent combustion. For example, combustion in homogeneous charge spark-ignition engines or in lean-burn gas turbines occurs under premixed conditions. In contrast, combustion in a diesel engine or in furnaces essentially takes place under nonpremixed or partially premixed conditions.

In the spark-ignition engine, fuel and oxidizer are mixed by turbulence for a sufficiently long period of time before the electrical spark ignites the mixture. The deposition of electrical energy from the spark ionizes the gas and heats it to several thousand degrees Kelvin. At temperatures above one thousand degrees Kelvin chemical reactions are initiated. These generate a flame kernel that grows at first by laminar, then by turbulent flame propagation. The turbulent burning velocity and its prediction from first principles will play a central role in the chapter on premixed turbulent combustion.

In stationary lean-burn gas turbines that have recently been developed for power generation, the fuel is prevaporized and premixed with air before entering into the combustion chamber. To homogenize the temperature field and thereby reduce emissions, in particular those of NO_x, turbulent mixing is very strong and dominates the combustion process. In the postflame region mixing with secondary air reduces the temperature to levels that are low enough not to destroy the turbine blades downstream of the exhaust. The reduction in temperature also freezes the NO_x formation in the postflame region.

In the rich-to-lean-burn gas turbines used in aircraft engines, liquid fuel is injected into the combustion chamber where it evaporates and burns in a turbulent diffusion flame, which is stabilized by swirl and recirculation. As in lean-burn gas turbines secondary air is mixed into the product stream of the flame to oxidize the remaining hydrocarbons, CO, and soot and to reduce the temperature at the exhaust.

In the diesel engine, several liquid fuel sprays are injected into hot compressed air; the fuel evaporates and mixes partially with the air before auto-ignition occurs. The auto-ignition process happens quite randomly and independently at several locations within the sprays. These ignition kernels will then initiate the burnout of the partially premixed fuel–air mixture. The final burnout occurs essentially under nonpremixed conditions.

In furnaces, finally, gaseous, liquid, or solid fuels are injected separately from the air into the combustion chamber. The air may be preheated or partially diluted by hot exhaust gases. Once the mixture is ignited, the flame propagates toward the nozzle until it stabilizes at a distance, called the lift-off height, downstream of the nozzle. Partial premixing takes place in the region between the nozzle and the lift-off height and determines the stabilization of the turbulent flame. Further downstream, combustion again occurs under nonpremixed conditions.

Cambridge University Press
0521660823 - Turbulent Combustion
Norbert Peters
Frontmatter
More information

It is clear that in addition to premixed and nonpremixed combustion, partially premixed combustion plays, at least locally, an important role in practical applications. Another example for partially premixed combustion is the modern direct-injection spark-ignition engine where the charge is stratified such that the flame initiated at the spark propagates through a partially premixed inhomogeneous mixture.

A second criterion for the subdivision of turbulent combustion relates to the ratio of turbulent to chemical time scales. Because of chain-branching reactions, hydrocarbon oxidation occurs if the temperature is above a certain crossover temperature, but it ceases if the temperature falls below that temperature. The crossover temperature is defined as the temperature where the effects of chain-branching reactions just balance that of chain-breaking reactions. At ambient pressure this temperature lies between 1,300 K and 1,500 K for hydrocarbon flames but it increases with pressure. At temperatures lower than the crossover temperature, extinction occurs, which must in general be avoided in practical applications. Therefore, combustion engines typically operate safely apart from extinction at conditions where temperatures are high enough and chemical reactions occur rapidly. This is often referred to as fast chemistry.

Slow chemistry does not very often occur in practical processes. Although NO_x formation is a relatively slow process, it is nearly always linked to the fast chemistry of the main combustion reactions, since it depends on the presence of radicals. There are a few applications of slow oxidation chemistry just above the crossover temperature between chain-branching and chain-breaking reactions, for example low NO_x burners, which operate at temperatures where both oxidation and NO_x chemistry are relatively slow. This process has been called MILD combustion. An example is the MILD combustion mode, which will be discussed in Chapter 3.

The four chapters in this book are organized as follows:

In Chapter 1, after a general introduction, the more prominent current modeling approaches for turbulent flows with combustion will be presented. At the end of that chapter an overview of the existing models in terms of mixing and in terms of infinitely fast or finite rate chemistry will be presented.

In Chapter 2, which deals with premixed turbulent combustion, emphasis will be placed on a combustion model that uses the level set approach to determine the location of the premixed flame surface. Damköhler's regimes of large scale and small scale turbulence will be associated with the corrugated flamelets regime and the thin reaction zones regime, respectively. Finally, based on an equation for the flame surface area ratio, an expression will be derived for the turbulent burning velocity, valid in both regimes. Other models and experimental data will be discussed in the light of this formulation. Although the mathematics behind the level set approach is rather demanding, the author believes that it is necessary in order to capture the physics of a propagating premixed turbulent flame surface.

In Chapter 3, models for nonpremixed combustion will be presented. Emphasis is placed on models that are based on the mixture fraction as independent variable. The definition and the role of the mixture fraction will be discussed in detail. The derivation of the flamelet equations will be based on two-scale asymptotic arguments. Filtering of the mixture fraction field and that of the reactive scalars outside of the thin reaction zone will justify the use of flamelet equations in the entire available mixture fraction range. The flamelet model will be compared to experiments and other models used for nonpremixed turbulent combustion. Scaling laws for round turbulent jet flames including NO_x formation and the influence of buoyancy will be presented.

Chapter 4 is concerned with partially premixed combustion. The classical problem in partially premixed combustion is flame stabilization at the lift-off height in a turbulent jet diffusion flame, which will be discussed in detail. The key element of the instantaneous flame front is the triple flame structure. The level set formulation for premixed combustion and the mixture fraction formulation for nonpremixed combustion will be combined to obtain an expression for the turbulent burning velocity in partially premixed systems. This expression is validated with respect to its capability to predict lift-off heights of lifted turbulent diffusion flames.

Finally, in the epilogue the principles behind turbulent combustion modeling are emphasized.

The turbulence models used in the four chapters of this book rely on modeling procedures that were developed for nonreacting constant density flows. They are highly disputed even for those applications because they rely on empiricism and some kind of intuition supplemented by physical arguments. It will become clear that with combustion, empiricism and the number of necessary simplifications increase. This is reflected by the large variety of different combustion models that have been formulated and that are pursued and continuously improved by different groups in the combustion community. In some cases competing models are based on the same physical concepts, with different modeling strategies leading to different formulations. In other cases, the concepts are fundamentally different. For instance, Lagrangian models such as those used in the pdf transport equation model differ in their physical and mathematical formulation from classical flamelet models formulated in the Eulerian framework. As a consequence, if one needs to solve a combustion problem numerically, an a priori choice has to be made as to which model to use. This is regretable, since no model is infallible and certainly no single approach will provide definite answers to the large variety of problems in turbulent combustion.

In view of these difficulties one may be tempted to give up trying to model turbulent combustion and revert to direct numerical simulations (DNS). However, as pointed out by Bray (1996), "DNS are an extremely valuable research tool . . . from which much can be learned. . . . However, DNS cannot and will not meet the pressing need for improved predictive methods to aid . . . the design of practical high Reynolds number combustion systems." The reason for this lies in the large range of scales that would have to be resolved if a full numerical simulation were to be performed. Since combustion requires molecular mixing on the smallest scale of turbulence, the Kolmogorov scale, this scale and the even smaller scales of the thin reaction layers would have to be resolved. The inertial subrange between the integral scale ℓ and the Kolmogorov scale η extends typically over two orders of magnitude in engineering applications with combustion. The size of the combustion chamber L is estimated as at least one order of magnitude larger than the integral scale. Therefore there are at least three orders of magnitude between L and the mesh size Δ needed to resolve processes occuring at the Kolmogorov scale by a direct numerical simulation. With constant mesh sizes and a three-dimensional (3D) mesh this would result in at least 10^9 grid points, which makes such computations prohibitive for many years to come.

However, quite elaborate numerical codes using adaptive gridding to account for complex geometries have been developed in recent years and are commercially available. These codes use RANS (Reynolds averaged Navier–Stokes equations) models and resolve the flow by using mesh sizes of the order of the integral length scale ℓ. Industrial users of these codes naturally demand that they are also applicable to flows with combustion. This sets a framework for turbulent combustion models that is quite restrictive and may require compromises.

A way to improve the predictive capability of these models, in particular with respect to the flow field, is to employ large eddy simulations (LES) for flows with combustion. LES models employ a larger number of grid points to resolve the energy containing scales within the inertial subrange. It will be argued at the end of Chapter 1 that some RANS models, in particular flamelet models combined with the presumed shape pdf approach, can easily be extended to LES.

I am indebted to many friends and colleagues in the combustion community for sharing with me over the past twenty years their stimulating ideas on turbulent combustion. Their papers are referenced in this book to the best of my knowledge. The book could also not have been written without the thesis work of many of my students and collaborators who have amply contributed to many of the sections in Chapters 2 to 4. That work has been funded generously by the Deutsche Forschungsgemeinschaft, which is gratefully acknowledged. Early versions of the manuscript have received critical reading by Bill Ashurst, Bernd Binninger, Philip de Goey, Johannes Janicka, Alain Kerstein, Rupert Klein, Moshe Matalon, Heinz Pitsch, Martin Oberlack, Luc Vervisch, and many others. This has considerably improved the text and is also gratefully acknowledged. Last but not least, I want to thank Beate Dieckhoff for her considerate and careful preparation of the manuscript.