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Turbulent Reacting Flows

Editors: P.A. Libby and F.A. Williams

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Turbulent Reacting Flows

Edited by P. A. Libby and F. A. Williams

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With 38 Figures

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Preface

Fluid mechanical turbulence is one of the most challenging fields of engineering science, rich in problems involving theory and experiment and having fundamental and applied significance. When chemical reactions occur in turbulent flows as is the case in many devices involving combustion, the challenge takes on a new dimension; the broad field of fluid mechanical turbulence is joined with another area of fluid mechanics, aerothermochemistry, which relates to the coupling between fluid dynamics, thermodynamics, and chemistry. There result sublimely complex problems involving the interaction of turbulent motions with the chemical and thermodynamic behavior associated with combustion. It is the purpose of this volume to provide background material that is needed to unravel the essentials of these complexities and interactions and to summarize recent theoretical approaches that have been developed in the field.

Turbulent reacting flows have attracted increased interest in recent years. The requirements of increased combustion efficiency and decreased pollutant emissions from a variety of devices, from power plants to jet engines, and the introduction of new devices such as the gas dynamic laser have led to the need for improved methods of prediction and calculation for turbulent flows involving chemical reactions. This increase in interest has led to a series of specialized meetings, workshops, publications, etc. References to the literature resulting from this activity will appear in the various chapters which follow. However, the field of turbulent reacting flows is in such a state of flux that it is difficult for a research worker, familiar to some extent with the essential background ingredients, fluid mechanics, turbulence, and aerothermochemistry, to gain perspective on our understanding of turbulent combustion and on our current capabilities to predict the structure of turbulent reacting flows. There thus appears a need for a tutorial treatment of the field.

In a book devoted to such a specialized field as turbulent reacting flows appropriate background knowledge must be assumed. Thus our exposition presumes that the reader has some knowledge of fluid mechanical turbulence and of aerothermochemistry; in Chap. 1 we suggest a few books providing this requisite background. With this knowledge as a foundation the present volume is self-contained and may be used as a textbook for a graduate course in mechanics, applied physics, or engineering or as an introduction to a new research area for the reader. One of our goals is to set forth the variety, challenge, and importance of the problems in turbulent reactant flows and thus to encourage research workers to enter the field.

The contents of the book are proscribed in another fashion. Many problems in turbulent combustion involve the injection of liquid or solid fuels into oxidizing gas streams. In these situations the combustion processes are accompanied by vaporization and/or sublimation and thus by additional complications. Similar remarks pertain to radiative transfer in turbulent reacting flows; in many flows involving combustion radiation from particles arising from incomplete combustion of injected solid fuel, from condensed-phase products of combustion, from refractory impurities contained in fuels, or from the nucleation of carbon in portions of the flow with excess fuel can provide significant energy transfer. With respect to both of these complications we shall limit discussion to a presentation in Chap. 6 of current entries into the literature on these largely untouched problems.

Throughout, our exposition emphasizes the fundamental bases and theoretical aspects of each topic. Experimental results and occasionally, in an idealized sense, the means to obtain them are introduced in order to reinforce the physical interpretation of a theoretical notion, to guide theoretical developments, e.g., in the introduction of models to close the describing equations, and to indicate the accuracy of theoretical prediction. We note that the application of experimental techniques to turbulent combustion is a separate discipline outside the scope of the present volume.

Chapter 1 sets the foundations of subsequent, more specialized discussions and reviews the general theoretical basis for the study of turbulent reacting flows in the context of combustion. It also establishes the notation used in the remainder of the book. Chapter 2 also has an introductory nature; it relates to the problems of an applied and practical nature which are of technological interest and which conceivably can be clarified and elucidated by the study of turbulent combustion. At this juncture the reader should have gained a sense of the complexities involved in the most general cases of turbulent combustion and will be prepared in the best tradition of the engineering sciences to deal with limited cases which, because of their nature, are amenable to facilitated treatment. Accordingly, Chaps. 3 and 4 will discuss the cases of nonpremixed and premixed reactants, respectively. Since there are practical situations which closely correspond to these two limits, their consideration is not of only academic interest. Throughout these chapters repeated use will be made of the notion of probability density functions in guiding the reader's perception of the phenomena involved and in developing suitable models and approximations. These functions relating to one or more fluid mechanical variables at each spatial location can be considered to play a more fundamental role than is suggested by such uses. In fact if a direct attack on the problem of describing turbulent reacting flows via the probability density function were feasible, many of the problems we discuss would be readily solvable; this is far from true, but certain limited problems can be attacked in this direct fashion, and Chap. 5 describes this approach and the problems involved in its extension.

Of necessity the flows treated in Chaps. 3–5 will be relatively idealized. Although many useful results are obtained from analyses of these simplified situations, there are flows of applied interest which do not lead themselves to these indications but rather involve in a significant way some of the effects which have been neglected. In addition, the current state of flux of the subject of turbulent reacting flows is manifest by several novel approaches whose thorough discussion would be inappropriate in a tutorial volume. However, attention should be called to them because of the difficulties and limitations associated with the more developed approaches emphasized in the various chapters. Finally, there are topics excluded from our exposition since they lie beyond the possible scope of this volume even though they are relevant to the study of turbulent reacting flows. In Chap. 6 we offer comments on aspects of turbulent reacting flows generally disregarded in Chaps. 3–5, on novel and developing approaches to the subject and on outstanding problems. References providing entries to the relevant literature of these topics are given in order to stimulate further interest and the additional research required to overcome current difficulties and limitations.

Because of the variety and complexity of the problems associated with turbulent reacting flows, their study can involve sophisticated techniques of applied mathematics and of experimental methods. Our approach is to emphasize the engineering and physical aspects of the subject, referring wherever indicated by exposition to experimental results and experimental methods and to problems of interest to applied mathematicians. Our hope is to provide a perspective of, and to stimulate interest in, a challenging and important field.

Our research on turbulent reacting flows has been supported over a period of several years by the Office of Naval Research as part of Project SQUID and by the Air Force Office of Scientific Research. This volume is a consequence of our research interests and we therefore gratefully acknowledge the contribution of these agencies. We also note with thanks the contributions of Ms. Barbara Hanson in the preparation of the manuscript of the Preface and of Chaps. 1 and 6.

La Jolla, July 1980

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Cavitation and Inhomogeneities in Underwater Acoustics

Proceedings of the First International Conference Göttingen, Fed. Rep. of Germany, July 9–11, 1979
Editor: W. Lauterborn

1980. 192 figures, 6 tables. XI, 319 pages
(Springer Series in Electrophysics, Volume 4)
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Hydrodynamic Instabilities and the Transition to Turbulence

Editors: H. L. Swinney, J. P. Gollub

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Y. I. Ostrovsky, M. M. Butusov,
G. V. Ostrovskaya

Interferometry by Holography

1980. 184 figures, 4 tables. X, 330 pages
(Springer Series in Optical Sciences, Volume 20)
ISBN 3-540-09886-0

Contents:
General Principles: Interference of Light. Optical Interferometry. Holography. Holographic Interferometry. – Experimental Techniques: Light Sources. Hologram Recording Materials. Setups. Experimental Aspects. – Investigation of Transparent Phase Inhomogeneities: Features of Holographic Interferometry of Transparent Objects. Sensitivity of Holographic Interferometry and Methods of Changing It. Holographic Diagnostics of Plasma. Use of Holographic Interferometry in Gas-Dynamic Investigations. – Investigation of Displacements and Relief: The Process of Interference-Pattern Formation in Holography. Methods of Interpreting Holographic Interferograms when Displacements are Studied. Investigation of Surface Relief. Flaw Detection by Holographic Interferometry. – Holographic Studies of Vibrations: Influence of Object Displacement on the Brightness of the Reconstructed Image – The Powell-Stetson Method. The Stroboholographic Method. Phase Modulation of the Reference Beam. Determining the Phases of Vibrations of an Object.

Turbulence

Editor: P. Bradshaw

2nd corrected and updated edition. 1978.
47 figures, 4 tables. XI, 339 pages
(Topics in Applied Physics, Volume 12)
ISBN 3-540-08864-4

Contents:
P. Bradshaw: Introduction. – *H.-H. Fernholz:* External Flows. – *J. P. Johnston:* Internal Flows. – *P. Bradshaw, J. D. Woods:* Geophysical Turbulence and Buoyant Flows. – *W. C. Reynolds, T. Cebecci:* Calculation of Turbulent Flows. – *B. E. Launder:* Heat and Mass Transport. – *J. L. Lumley:* Two-Phase and Non-Newtonian Flows.

H. Haken

Synergetics

An Introduction

Nonequilibrium Phase Transitions and Self-Organization in Physics, Chemistry and Biology.

'Springer Series in Synergetics'

2nd enlarged edition. 1978. 152 figures, 4 tables. XII, 355 pages
ISBN 3-540-08866-0

Contents:
Goal. – Probability. – Information. – Chance. – Necessity. – Chance and Necessity. – Self-Organization. – Physical Systems. – Chemical and Biochemical Systems. – Applications to Biology. – Sociology: A Stochastic Model for the Formation of Public Opinion. – Chaos. – Some Historical Remarks and Outlook.

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Ocean Acoustics

Editor: J. A. DeSanto

1979. 109 figures, 5 tables. XI, 285 pages
(Topics in Current Physics, Volume 8)
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Contents:
J. A. DeSanto: Introduction. – *J. A. DeSanto:* Theoretical Methods in Ocean Acoustics. – *F. R. DiNapoli, R. L. Deavenport:* Numerical Models of Underwater Acoustic Propagation. – *J. G. Zornig:* Physical Modeling of Underwater Acoustics. – *J. P. Dugan:* Oceanography in Underwater Acoustics. – *N. Bleistein, J. K. Cohen:* Inverse Methods for Reflector Mapping and Sound Speed Profiling. – *R. P. Porter:* Acoustic Probing of Space-Time Scales in the Ocean. – Subject Index.

Turbulent Shear Flows I

Selected Papers from the First International Symposium on Turbulent Shear Flows, The Pennsylvania State University, University Park, Pennsylvania, USA, April 18–20, 1977
Editors: F. Durst, B. E. Launder, F. W. Schmidt, J. H. Whitelaw

1979. 256 figures, 4 tables. VI, 415 pages
ISBN 3-540-09041-X

Contents:
Free Flows. – Wall Flows. – Recirculating Flows. – Developments in Reynolds Stress Closures. – New Directions in Modeling.

Turbulent Shear Flows II

Selected Papers from the Second International Symposium on Turbulent Shear Flows, Imperial College London, July 2–4, 1979
Editors: J. S. Bradbury, F. Durst, B. E. Launder, F. W. Schmidt, J. H. Whitelaw

1980. 310 figures. Approx. 410 pages
ISBN 3-540-10067-9

Contents:
Turbulence Models. – Wall Flows. – Complex Flows. – Coherent Structures. – Environmental Flows. – Index of Contributors.

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1. Fundamental Aspects

P. A. Libby and F. A. Williams

With 2 Figures

The basic equations that describe turbulent reacting flows usually are accepted to be the Navier-Stokes equations, suitably amplified to include chemical reactions, species conservation, and variable-property effects. This chapter offers an exposition of these equations. It opens with suggestions for background reading that may serve as a point of departure. After preliminary delimitation of the types of problems covered within this volume, it continues with a review of elements of fluid mechanical turbulence and of aerothermochemistry necessary for an understanding of the phenomena. This review includes establishment of notation; discussions of transport properties and of chemical kinetics; alternative approaches to probabilistic descriptions, such as time averaging, Favre averaging, and equations for evolution of probability-density functionals; specific turbulence topics of potential relevance to reacting flows, such as intermittency and spectral decompositions; nondimensionalizations resulting in similarity parameters that help to quantify limiting behaviors; methods for treatment of chemical reactions in turbulent reacting flows; and some discussion of methods of closure. The intent in this chapter is to set the stage for more detailed considerations that are given in subsequent chapters.

1.1 Background Literature

A variety of books are available for obtaining the appropriate background in fluid-mechanical turbulence. We especially recommend *Bradshaw* [1.1, 2] and *Tennekes* and *Lumley* [1.3] as providing a useful and practical focus. More extensive treatments are offered by *Hinze* [1.4] and by *Monin* and *Yaglom* [1.5]. Background information in aerothermochemistry and combustion may be obtained from the books by *Penner* [1.6] and by *Williams* [1.7], for example. More recent texts on combustion include those of *Strehlow* [1.8] and *Glassman* [1.9].

A current review of fluid mechanical turbulence is given by *Reynolds* [1.10]. Reviews on turbulent reacting flows have been prepared by *Hill* [1.11] and by *Libby* and *Williams* [1.12]. *Launder* and *Spalding* [1.13] and *Spalding* [1.14] provided entries into the current literature on the more application-oriented aspects of turbulence phenomenology.

1.2 Turbulence in Reacting Liquids and Gases

Liquids and gases constitute two limiting states of fluids which fundamentally exhibit very different properties. Although the present volume concerns chemical reactions in gases, the results are applicable to liquids in certain respects. Therefore an introductory discussion of the differences between liquids and gases seems warranted.

The most convincing justification for the use of the Navier-Stokes level of description of flows differs for liquids and gases. Most gases of interest are "dilute" in the kinetic-theory sense; the duration of molecular collisions is short compared with the time between collisions. By contrast, a molecule in a liquid experiences collisions most of the time. For dilute gases the kinetic theory is relatively well developed and provides the most convincing foundation from which the Navier-Stokes description can be derived. For liquids, complexities of dense-gas kinetic theory cause a phenomenological, continuum-mechanical derivation of the Navier-Stokes equations to be more satisfying than kinetic-theory derivations. Thus, the origins of the describing equations may be viewed as differing for the two limiting states.

When the starting point is phenomenological, no avenue is open for questioning the validity of the describing equations. In contrast, a derivation from kinetic theory can be challenged by questioning specific assumptions, such as molecular chaos, that are introduced during the derivation. Recently a few investigators have raised such challenges to Navier-Stokes turbulence for dilute gases (see, for example, [1.15]). The possibility of the existence of associated influences on turbulent reacting flows recently has been brought out by *Tsugé* and *Sagara* [1.16], who achieved agreement with anomalous experimental results on hydrogen–oxygen ignition by means of an analysis that is based on kinetic theory and that denies applicability of a Navier-Stokes level of description to certain experiments. Although the possibilities for failure of a Navier-Stokes description are interesting, this topic is too new and much too incomplete to be covered within the present volume. Therefore we adopt the classical viewpoint that, for gases as well as liquids, the basic equations underlying the description of turbulent reacting flows are the Navier-Stokes equations, and the probabilistic structures appropriate for such flows are to be erected upon those equations.

Given this identical level of description, there remain significant differences between liquids and gases experiencing chemical reactions. Aside from subsidiary influences such as buoyant convection, the density is essentially constant in a reacting liquid but changes substantially as a result of heat release for most reactions in gases (notably for all combustion reactions). This simplifies the dynamics of turbulent reacting flows for liquids, in that the turbulent behavior of the velocity field is unaffected by the chemistry. In contrast, for the turbulent reacting flows of interest in gases, the full interaction between turbulence and chemistry occurs: The turbulence influences the effective chemical behavior and the heat release associated with the exothermic chemical reactions alters the turbulence. In this respect, the problems addressed in the present volume are more complex than those of chemical reactions in turbulent liquids.

Offsetting this relative simplicity of liquids is a complication associated with molecular transport properties. In gases, diffusivities of heat, chemical species, and momentum all are of the same order of magnitude (with the possible exception of hydrogen which diffuses an order of magnitude faster than other species). However, in liquids the diffusivity of heat is large compared with that of momentum, which in turn is large compared with diffusivities of species. This introduces into the dynamics of turbulent mixing of liquids elements not found in turbulent mixing of gases (see for example, [1.17, 18]) and correspondingly may influence reaction dynamics in turbulent liquids. In many problems this complexity may be relatively insignificant; often it is thought that for sufficiently intense turbulence molecular transport is unimportant in comparison with turbulent transport. However, in general, studies of effects of large differences in molecular transport coefficients are well motivated primarily for liquids. Such effects are excluded from the present volume.

A final way in which turbulent reacting liquids behave more simply than turbulent reacting gases stems from the fact that reaction rates usually tend to be relatively high in liquids. This difference ultimately rests on the continual intermolecular collisions occurring in liquids, in comparison with the relatively rare intermolecular encounters of gases. The rapid reaction in liquids allows certain simplifications associated with the notion of "fast chemistry" to be applied more widely in liquids than in gases. This and the aforementioned constant-density property of liquids allow many of our considerations to apply to chemical reactions in turbulent liquids. In particular, one limiting case of reactions in gases, that involving highly dilute reactants undergoing fast chemistry, is directly applicable to reactions in liquids when large differences in coefficients of molecular transport are unimportant.

1.3 The Eulerian Viewpoint and Notation

Although there are specific processes, such as turbulent diffusion, in which clarification can be achieved through use of a Lagrangian viewpoint [1.3], complexities that arise in attempting to tie the coordinate system to fluid parcels in turbulent flows of general types usually lead to the adoption of the Eulerian viewpoint. Following this latter convention, we consider the behavior with time of the various quantities characterizing the flow at a fixed spatial point. These quantities are the components of velocity and the state variables, pressure, density, and concentrations of chemical species. Each of these quantities is considered to have associated with it an ensemble average or mean value, which may vary in space and time, and a fluctuation, which always depends on space and time and which typically varies much more rapidly than the mean.

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