Preface

Since its initial publication in 2001, many readers have commented that *Theoretical and Numerical Combustion* is useful in that it provides a coherent summary of research in a field where advances occur rapidly, especially in the area of numerical simulation. This Second Edition recognizes the research advances of the past four years. In addition, however, we acknowledge that the fast pace of research makes teaching combustion difficult, especially when the numerous prerequisites required to grasp the essence of modern combustion science are considered. Therefore, our two primary objectives in preparing this Second Edition were:

- to capture the most recent advances in combustion studies so that students and researchers alike can (hopefully) find the most essential information in this text; and
- to simplify, as much as possible, a complex subject so as to provide a reasonable starting point for combustion beginners, especially those involved in numerical simulations.

Obviously, numerical techniques for combustion are essential tools for both engineers and research specialists. Along with many of our colleagues, we strongly believe that this evolution toward more simulations is dangerous if it is not accompanied by a minimum expertise in combustion theory. Obtaining expertise in combustion theory and modeling is much more difficult than simply being able to run "off-the-shelf" codes for combustion. Yet, considering the enormous stakes associated with the design of combustion devices in terms of both economy and human safety, it is imperative that this deep understanding not be shortcut. We implore all members of the combustion community to strive to ensure that the capabilities and limitations of numerical simulations are well understood. We would like this book to continue to be one of the tools available to achieve this understanding. To accomplish this we have maintained our presentation of the basic combustion theories, and have sought to establish necessary connections and interrelationships in a logical and comprehensible way.

A major evolution of numerical combustion of the past few years is the development of methods and tools to study *unsteady* reacting flows. Two combined influences explain this trend; namely,

- Many of the present challenges in the combustion industry are due to intrinsically unsteady mechanisms: autoignition or cycle-to-cycle variations in piston engines, ignition of rocket engines, combustion instabilities in industrial furnaces and gas turbines, and flash-back and ignition in aero gas turbines. All these problems can be studied numerically, thus partially explaining the rapid growth of the field.

- Even for stationary combustion, research on classical turbulent combustion models (herein called RANS for Reynolds Averaged Navier Stokes) is being replaced by new unsteady approaches (herein called LES for Large Eddy Simulations) because computers allow for the computation of the unsteady motions of the flames. However, these new unsteady methods also raise new problems: for example, how are numerical results compared with experimental data, and what explains the deviations?

Major changes in the Second Edition actually reflect these evolutionary influences: the chapters on turbulent combustion and modeling (Chapters 4 through 6) incorporate recent advances in unsteady simulation methods. Chapter 8 has also been extensively modified to describe combustion/acoustics interaction. Chapter 10, an entirely new chapter, is devoted to important examples of LES which illustrate the present state of the art in numerical combustion while discussing the specificities of swirled flows.

This book can be read with no previous knowledge of combustion, but it cannot replace many existing books on combustion (Kuo[285], Lewis and Von Elbe[304], Williams[554], Glassman[193], Linan and Williams[315], Borghi and Destriau[51], Peters[398]) and numerical combustion (Oran and Boris[383]). We concentrate on what is not in these books: i.e. giving to readers who know about fluid mechanics all the information necessary to move on to a solid understanding of numerical combustion. We also avoid concentrating on numerical methods for fluid mechanics. Information on Computational Fluid Dynamics (CFD) may be found in Roache[448], Anderson[8], Hirsch[227], Oran and Boris[383], Ferziger and Perić[167] or Sengupta[477]. This text concentrates on which equations to solve and not on how to solve them.

Two important topics are also absent from the present edition:

- The presentation is limited to deflagrations, i.e. to flames with low speed. Detonations constitute a different numerical challenge which is not considered here (see Oran and Boris[383]).

- The chemistry of combustion is also a topic which requires a book (or many) in itself. This text does not try to address this issue: the construction of chemical schemes and their reduction and validation are not discussed here. The impact of chemical schemes on reacting flow computations, however, is discussed; especially in the field of turbulent combustion. Recent progress in this field, both at the fundamental level and for practical applications, has changed the way industrial combustion systems are being designed today. The important numerical tools needed to understand this evolution are presented.

The Second Edition is now organized as follows:

- Chapter 1 first describes the conservation equations needed for reacting flows and reviews different issues which are specific to the numerical resolution of the Navier Stokes equations for a multi-species reacting flow. Tables summarizing the main conservation forms used in numerical combustion codes are provided. Specific difficulties associated with reacting flows are also discussed: models for diffusion velocities, possible simplifications for low-speed flames and simple chemistry approximations. Compared to the previous edition, the discussion about diffusion velocities was revised, clearly stating exact formulations and usual approximations (§1.1.4).

- Chapter 2 provides a short description of numerical methods for laminar premixed flames. It also includes a summary of many significant theoretical results which are useful for numerical combustion. Most of these results come from asymptotic theory. They are given here to not only provide an understanding of the results and limitations of numerical combustion codes, but also to provide insight into how to initialize them, determine necessary grid resolutions, and to verify their results. Extended definitions and examples of flame speeds, flame thicknesses and flame stretch are discussed.

- Chapter 3 introduces laminar diffusion flames and two specific concepts associated with such flames: mixture fraction and scalar dissipation. Asymptotic results and the structure of the "ideal" diffusion flame are used to provide an accurate picture of the phenomenology of these flames before computation.

- Chapter 4 introduces the basic concepts used to study turbulent combustion. Elementary concepts of turbulence and flame/turbulence interaction are described. Averaging and filtering procedures are discussed. A classification of the different methods (RANS: Reynolds Averaged Navier Stokes, LES: Large Eddy Simulation, DNS: Direct Numerical Simulation) used in numerical combustion for turbulent flames is given. New sections have been added to discuss the incorporation of complex chemistry features in turbulent flame computations (§4.8), the classification of physical approaches to model turbulent combustion phenomena according to recent papers (§4.5.5), and the comparison between LES and experimental data (§4.7.7).

- Chapter 5 presents turbulent premixed flames. After a description of the main phenomena characterizing these flames, a review of recent results and theories is presented for RANS, LES and DNS approaches. Implications for turbulent combustion computations are discussed. The close relations between all numerical techniques used in the last ten years (especially DNS results used to develop RANS or LES models) are emphasized.

- Chapter 6 presents turbulent diffusion flames. These flames present even more complexities than premixed flames and numerical investigations have recently helped to uncover many of their specificities. Models are also very diverse. The topology of diffusion flames is first described and RANS methods used for turbulent non premixed combustion are classified for CFD users. Recent advances in the field of LES and DNS are also described.

- Chapter 7 addresses the problem of flame/wall interaction. This issue is critical in many combustion codes. Asymptotic results and DNS studies are used to illustrate the main characteristics of this interaction. Models including this interaction in RANS codes are described. Since the presence of a flame strongly modifies the turbulence as well as the density and the viscosity near walls, models for wall friction and heat transfer in reacting flows are also discussed.

- Chapter 8 describes a series of theoretical and numerical tools used to study the coupling phenomena between combustion and acoustics. This coupling is the source of not only noise, but also of combustion instabilities which can significantly modify the performances of combustors and sometimes lead to their destruction. Basic elements of acoustics in non reacting flows are described before extending acoustic theory to reacting flows. This chapter then focuses on three numerical tools for combustion instability studies: (1) one-dimensional acoustic models to predict the global behavior of a full combustion system submitted to longitudinal waves, (2) three-dimensional Helmholtz codes to identify possible acoustic modes in a burner and (3) multi-dimensional Large Eddy Simulation codes to investigate the detailed response of the combustion chamber itself which is a critical building block for acoustic models. Examples of applications with complex geometries are provided in Chapter 10.

- Chapter 9 presents recent techniques to specify boundary conditions for compressible viscous reacting flows. Modern simulation techniques (LES or DNS) as well as recent applications of CFD (such as combustion instabilities described in Chapter 8) require elaborate boundary conditions to handle unsteady combustion and acoustic waves as well as to adjust for numerical schemes which do not provide large levels of dissipation. This chapter provides an overview of such methods and offers a list of test cases for steady and unsteady flows which can be used in any code.

- The new Chapter 10 describes three very recent applications of large eddy simulations to complex-geometry swirled combustors both to predict the mean flow structure and to analyze unsteady hydrodynamic and acoustic phenomena. These examples provide information on the flow physics of these combustors while also demonstrating how recent numerical tools can be applied today.

To assist the reader, this book uses two distinctive pedagogical devices throughout. First, fundamental and frequently used formulae are boxed for easy identification. Second, an innovative citation system has been adopted to provide rapid access to a comprehensive set of references. In addition, unsteady flow animations are available on the web to simplify the description of certain unsteady phenomena in Chapter 10.

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