Preface

This text presents basic techniques and recent progress in the field of numerical combustion. The complexity of reacting flows often limits our ability to handle such phenomena without the help of computers. As a result, numerical techniques for combustion have become essential tools for engineers as well as for research specialists. This state of affairs brings two comments:

- First, the development of “off-the-shelf" codes for numerical combustion leads many users to believe that these may be employed without knowledge of combustion theory. This is a dangerous mistake. Proper utilization of combustion codes cannot be achieved at the moment without understanding combustion basics. Unfortunately, these basic theories are often presented in highly specialized texts and non-experts are reluctant to spend the time needed to understand and use theoretical results. We attempt to identify and present these complex interrelationships in a logical and comprehensible way.
- Second, the numerics of combustion are difficult because they gather the specificities of fluid mechanics and of chemical systems. In general, solving for combustion means solving for the flow and for the chemical species. And since flow and species distributions are strongly coupled the resolution must be simultaneous. Numerical schemes derived for non-reacting flows cannot be extended in a straightforward manner to reacting flows: for these flows, heat release induces changes in density, viscosity and diffusion coefficients which change the requirements needed in the numerical method. The existence of very stiff chemical source terms in the species and energy equations is in itself an additional and crucial problem.

There are many excellent books on both combustion (Kuo[259], Lewis and Von Elbe[277], Williams[486], Glassman[179], Linan and Williams[288], Borghi and Destriau[51], Peters[356]) and numerical combustion (Oran and Boris[344]) and our aim is not to duplicate these books. Instead, 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 comcombustion. We also avoid concentrating on numerical methods for fluid mechanics. Information on Computational Fluid Dynamics (CFD) may be found in Roache[400], Anderson[8], Hirsch, Oran and Boris[344] or Ferziger and Peric[154]. This text concentrates on which equations to solve and not on how to solve them.

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[344]). 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.

This text is 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.

- 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 or verify their results. Extended definitions and examples of flame speeds, flame thicknesses or flame stretch are given and 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.

- 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. Basic elements of acoustics in non reacting flows are described before extending acoustic theory to reacting flows. This chapter then focuses on two 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 and (2) multi-dimensional Large Eddy Simulation codes to investigate the detailed response of the combustion chamber itself which is a critical building block for the one-dimensional acoustic models.
- 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 gives the basis of such methods and provides a list of test cases for steady and unsteady flows which can be used in any code.

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.

Thierry POINSOT
Institut de Mécanique des Fluides
UMR CNRS/INP/UPS 5502
Institut National Polytechnique
de Toulouse/ENSEEIHT

Denis VEYNANTE
Laboratoire E.M2.C.
UPR CNRS 288
Ecole Centrale Paris