von Karman Institute Lecture Series
"Turbulence and Combustion"
19–23 March 2001, Rhode-Saint-Genèse, Belgium

Applications of Turbulent Combustion Modeling

By Daniel C. Haworth

Department of Mechanical & Nuclear Engineering
The Pennsylvania State University
University Park, PA 16802–2321
USA
dch12@psu.edu

The emphasis in this overview of applications of turbulent combustion modeling is device–scale computational fluid dynamics (CFD). CFD–based modeling is playing an increasingly important role in combustion–system analysis and design. A review of the underlying governing equations, and the manipulations and simplifications that lead to a tractable equation set suitable for engineering calculations, is provided first. Four topics in turbulent combustion modeling then are highlighted: direct numerical simulation of turbulent reacting flows, hybrid models for mixed–mode combustion processes, storage/retrieval schemes to accommodate detailed chemical kinetics, and modeling of an archetypical turbulent reacting flow: a turbulent non–premixed jet flame. This is followed by examples of several device–scale applications: reciprocating–piston internal–combustion engines, gas–turbine combustors, fires, and chemical reactors. These examples serve to illustrate the diversity of phenomena that comprise turbulent combustion, and the utility of combustion modeling. They also serve to demonstrate strengths and shortcomings of current modeling approaches, and thereby to motivate directions for future research and applications. The final section includes a few comments on topics that were not covered. And finally, a few near–term predictions for the future of turbulent combustion modeling are offered.

---

1. Introduction

Turbulent combustion is an important and timely subject in engineering science. Many of the most urgent energy efficiency and pollutant emission issues worldwide are related to the conversion of chemical energy to sensible energy (heat) via a combustion process in a turbulent flow environment. Combustion devices of practical interest include stationary and automotive reciprocating–piston engines, stationary and aircraft gas–turbine combustors, industrial burners, and chemical production/processing reactors. The combustion process in such devices usually is characterized by complex turbulence–chemistry interactions that span multiple combustion regimes: premixed flame propagation, mixing–controlled burning, and chemical–kinetics–controlled processes may occur simultaneously within a single device. A wide range of flow speeds (Mach numbers) may be relevant. Two–phase flows (liquid fuel sprays), heterogeneous combustion (walls/catalysts), and radiation heat transfer (large–scale systems, sooting flames) often are important. This complex turbulent aero–thermo–chemistry occurs in tortuous three–dimensional geometric configurations. And the prediction of key trace species (reaction intermediates, pollutants, and/or signature species) may require consideration of tens–to–hundreds of chemical species and hundreds–to–thousands of chemical reactions.

Hydrodynamic turbulence by itself remains one of the outstanding fundamental problems of classical physics; the additional complexity of chemical reaction multiplies the difficulty by many orders of magnitude. The coupling among complex chemical kinetics, multi–component molecular transport, and hydrodynamic turbulence remains an unresolved fundamental problem. And the extent to which combustion engineers can improve performance while simultaneously reducing the fuel consumption and emissions of engineering combustion devices is limited by the design/analysis tools that they have at their disposal. Current computational fluid dynamics (CFD)–based tools are useful, but remain limited in their capacity to deal simultaneously with three–dimensional time–dependent turbulent flow, realistic chemistry and turbulence–chemistry interaction, multiple–phase/heterogeneous systems, radiation heat transfer and turbulence/radiation interaction, and arbitrary geometric configurations. At the same time, relatively few well–characterized high–resolution experimental datasets are available in parameter ranges

and geometric configurations of practical interest. Such data are essential to establish the underlying physics, to develop and calibrate models, and to validate codes.

The emphasis here is device–scale CFD–based modeling for practical turbulent combustion systems. Given the rapid advances in turbulent combustion modeling and the dramatic growth in CFD capability over the past 10 to 15 years, a comprehensive treatment is not possible and will not be attempted. The scope is limited to: 1) a review of fundamental aspects to provide the foundation necessary for developing and interpreting models; 2) examples of recent developments that offer substantial promise for device–scale turbulent combustion modeling; and 3) a sampling of device–scale applications to illustrate the nature and variety of issues that characterize practical combustion systems, to provide insight into the strengths and shortcomings of current modeling approaches, and to motivate future research directions and new areas of application. While multiple–phase, heterogeneous combustion processes and radiation heat transfer are of increasing practical interest, the emphasis here is primarily (although not exclusively) on gas–phase combustion processes for ideal–gas mixtures, without radiative heat transfer. And while there is growing interest in chemical systems beyond the hydrocarbon–fuel/air–oxidizer systems that dominate in engineering energy conversion applications, the focus remains primarily (although not exclusively) on hydrocarbon/air systems.

The material is organized as follows. An equation–based overview of turbulent aero–thermo–chemistry is presented in the following section. In Section 3, recent developments in turbulent combustion modeling are presented and discussed. Section 4 provides several examples of device–scale applications of turbulent combustion modeling. And in the final section, a few comments are given on physical phenomena and modeling approaches that were not dealt with in previous sections, and some near–term predictions are offered on the future of turbulent combustion modeling for engineering applications.

2. Turbulent Aero–thermo–chemistry

Salient aspects of turbulent combustion and its modeling are reviewed. This material is included to ensure continuity and self–consistency; more complete treatments are available elsewhere (e.g., Veynante & Vervisch 2001). The present approach emphasizes the central role played by probability density functions (PDF's) in turbulent combustion. The principal equations governing a multicomponent reacting gas mixture are introduced first. These equations must be simplified to deal with turbulent chemically reacting flows. To that end, a one–point statistical approach is reviewed, based on probability density functions; PDF and moment transport equations are presented. Finally, the modeling of key unclosed terms in the PDF and moment equations is discussed.

2.1. *The PDE's of Multicomponent Reacting Flows*

The partial differential equations (PDE's) governing a multicomponent chemically reacting system comprising N_S chemical species are expressed here using Cartesian tensor notation. A Roman index denotes a component of a three–dimensional vector (e.g., $i = 1, 2, 3$), a Greek index denotes a chemical species (e.g., $\alpha = 1, 2, \ldots, N_S$), and the usual summation convention applies over repeated Roman indices within a term. Here $\underline{u}$ denotes velocity, $\underline{Y}$ the mass fractions of the N_S chemical species, and h the enthalpy. Mixture mass density is ρ, pressure is p, body force (per unit mass) is $\underline{g}$, and $\underline{\underline{\tau}}$, $\underline{J}^\alpha$, and $\underline{J}^h$, denote, respectively, the viscous stress tensor and the molecular fluxes of species and enthalpy. The molar chemical production rate and molecular weight for species α are $\dot{\omega}_\alpha$ and W_α. The volume rate of heating due to radiation (absorption minus emission) is $\dot{Q}_{rad}$:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} &= 0 \quad , \\
\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_i} &= \frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial p}{\partial x_j} + \rho g_j \quad (j = 1, 2, 3) \quad , \\
\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho Y_\alpha u_i}{\partial x_i} &= -\frac{\partial J_i^\alpha}{\partial x_i} + \rho S_\alpha \quad (\alpha = 1, 2, \ldots, N_S) \quad , \\
\frac{\partial \rho h}{\partial t} + \frac{\partial \rho h u_i}{\partial x_i} &= -\frac{\partial J_i^h}{\partial x_i} + \frac{Dp}{Dt} + \tau_{ij} \frac{\partial u_j}{\partial x_i} + \dot{Q}_{rad} \quad ,
\end{aligned} \tag{2.1}$$

where $\rho S_\alpha = W_\alpha \dot{\omega}_\alpha$. The enthalpy (or energy, or temperature) equation can be written in a number of alternative forms (Kuo 1986). The present form is appropriate for the absolute enthalpy (sum of sensible