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Applications of Turbulent Combustion Modeling

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Multidimensional modeling (computational fluid dynamics - CFD) is playing an increasingly important role in advanced combustion-system development. Approaches that have the potential to address key performance, efficiency, and emissions issues for current and future engineering combustion systems are emphasized in this overview: in particular, models and methods that can accommodate multiple combustion regimes and detailed chemical kinetics. 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. Distinctions among direct numerical simulation (DNS), Reynolds-averaged simulation (RAS), and large-eddy simulation (LES) are drawn. The roles of DNS in extracting fundamental physical insight and in developing and calibrating engineering models are highlighted through examples of DNS for canonical configurations. This is followed by applications of RAS, LES, and DNS to laboratory-scale turbulent flames for model development and validation. Examples of device-scale applications of turbulent combustion modeling (RAS and LES) are discussed for reciprocating-piston internal-combustion engines, gas-turbine combustors, 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 some observations on progress in turbulent combustion modeling over the past 10-15 years, current trends in modeling, and near-term predictions for the future of turbulent combustion modeling.

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1. Introduction

Turbulent combustion is an important and timely subject in engineering science. Many of the most urgent energy efficiency, global climate change, 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 internal-combustion engines, stationary and aircraft gas-turbine combustors, and industrial burners. 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. Multiple-phase flows (liquid fuel sprays, solid particles), heterogeneous combustion (walls/catalysts), and radiation heat transfer (high-pressure and/or large-scale systems, sooting flames) often are important. This complex turbulent aero-thermo-chemistry may occur in tortuous three-dimensional geometric configurations. And the prediction of local extinction/ignition and 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, chemical kinetics, and thermal radiation individually are among the most challenging fundamental and practical problems of computational science and engineering. In chemically reacting tur-