Combustion subgroup: overview

High-fidelity numerical simulation of turbulent combustion has become an important tool for guiding the design of energy and propulsion systems in aerospace, transportation and various other industrial sectors. Ever-increasing demands for clean and sustainable energy have recently been driving combustion research toward carbon-free technologies and efficient engine design—"to burn less but burn better," as phrased by Thierry Poinsot.

The research topics addressed in the CTR Summer Program 2002 Combustion subgroup highlight this trend. Targeted application systems of the six projects cover lean hydrogen combustors, high-temperature gas-turbine engines, rotating detonation engines (RDEs) and iron-powder combustors. Modeling of these systems may require not only the extension of previous simulation tools to accommodate new regimes of flows, chemistry and/or geometries but also deep insights into underlying flow physics, which can be unique to the fuels and engines considered therein. To this end, each project primarily focused on physics-based modeling and analysis of flames and combustion that are relevant to the targeted systems.

Hydrogen is attracting considerable attention as a low-emission fuel. Flames of lean hydrogen/air mixtures tend to be thermodiffusively unstable due to strong differential diffusion. The instability can lead to small-scale flame wrinkling, which may influence the fuel consumption rate and NO_x production. Previous simulation tools, which do not account for the effects of instability, may not provide accurate predictions of the efficiency and pollutant emission of application systems.

Three projects addressed hydrogen flames with an emphasis on the thermodiffusive instability. Berger *et al.* developed a subgrid-scale model for large-eddy simulation (LES) of premixed hydrogen flames, which accounts for the instability in the flamelet-progresses variable framework. Manifold optimization was performed to accurately parameterize the subgrid-scale probability density functions of transport variables. *A-priori* analysis of this model using three-dimensional (3D) direct numerical simulation (DNS) data of canonical slot-burner flames showed favorable results. Wen *et al.* performed 2D and 3D DNS of canonical, thermodiffusively unstable premixed hydrogen flames to characterize the NO_x formation. Results show that 3D simulation is crucial to accurately predicting the NO_x production. A reaction path analysis was conducted to identify relevant reaction pathways. Moreover, the performance of a flamelet model in predicting the NO_x species was evaluated *a-priori*. The model accuracy was found to critically depend on the local flame curvature. Aniello *et al.* developed a dynamic thickened-flame (TF) model for LES of premixed hydrogen flames to account for the instability. The effects of subgrid-scale flame wrinkling and modifications of the consumption rate were parameterized to express the efficiency function, with the aid of DNS data provided by Berger *et al.*. The TF model was used to simulate flames in realistic swirl combustors. Results were compared with recent experiments.

RDEs are promising for propulsion and energy systems due to their high potential efficiencies and compact designs. The criteria of detonation-to-deflagration transition (DDT) in realistic RDEs are elusive. Elasrag *et al.* introduced a characteristic Damkhler number (Da) to distinguish detonation and deflagration regimes in hydrogen/slash air flames. The Da is defined in terms of the H radical that was identified as a suitable ignition indicator in chemical explosive mode analysis of 1D canonical flames. This criteria was

applied to various simulation data of detonation flames, including those of AFRL 6-inch RDE.

The operating temperature of gas-turbine engines is continuously increasing to improve combustion efficiency. Accurate predictions of the temperature distribution on the combustor wall are crucial for cooling design. Cui & Bose performed coupled wall-modeled LES and conjugate heat transfer analyses of the full-scale NASA Energy Efficient Engine combustor. The simulated temperature distribution on a perforated cooling liner in the combustor showed favorable agreements with previous measurements.

Finally, iron powders produced as industrial byproducts can be considered to be carbon-free renewable fuels. Combustion processes of gaseous turbulent flows laden with nano-sized ion particles have not been fully understood. Ravi *et al.* introduced an Eulerian-Lagrangian framework to resolve the fine-scale flow field near individual reacting particles by using a distribution kernel method. A grid-convergence study was performed by simulating the reaction of a single isolated particle. A canonical 2D simulation was performed to capture the formation of discrete flames in a stoichiometric, dilute particle/air mixture.

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