Advanced Scientific Computing Research
FY 2006 Accomplishment

Simulation of ultra-lean turbulent premixed hydrogen flames

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Summary

A dominant factor determining the burning rate of a premixed turbulent flame is the degree to which the flame is wrinkled by turbulence. However, in ultra-lean premixed hydrogen flames, interactions between turbulence, transport and chemistry lead to local extinction pockets and the simple relationship between flame surface area and burning rate breaks down. Detailed studies coupling large-scale computing with laboratory experiments are helping to unravel the complex interactions between turbulence and lean premixed flame chemistry.

Background

Recent interest in alternative fuels such as hydrogen or syngas has sparked the development of high-efficiency, low emissions lean premixed burners that can operate over a broad range of fuels. The feasibility of these systems in an industrial setting requires the development of robust flame stabilization techniques, and may be strongly impacted by detailed coupling between turbulence and chemistry and transport processes at the flame surface.

Figure 1 shows measurements of an ultra-lean premixed hydrogen flame stabilized on an experimental turbulent swirl burner. The Planar Laser-Induced Fluorescence (PLIF) signal for the OH flame radical serves as an experimental marker of local combustion intensity. The gaps shown here in the OH signal indicate local extinction driven by differential species diffusion.

Conventional approaches to the analysis of turbulent premixed combustion experiments are based on a theoretical model that treats the flame as an interface propagating

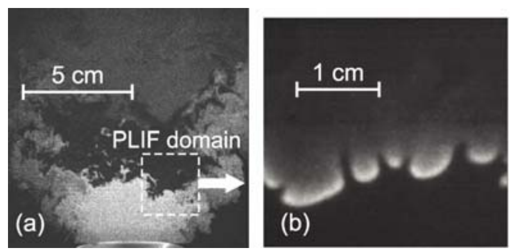

Figure 1: *(a) Mie scattering image, and (b) OH-PLIF of a lean premixed turbulent hydrogen flame in a 5cm diameter experimental low-swirl burner. Images courtesy R. Cheng and I. Shepherd, LBNL Combustion Laboratory.*

through the fluid. In essence, this “thin flame” approach separates the details of the flame structure from the background fluid mechanics. When local extinction occurs, as in the example above, the thin flame model is not applicable—the flame surface breaks. Detailed analysis of the underlying processes requires more insight than standard experimental diagnostics can reveal.

Approach

We are using detailed simulations to augment experimental diagnostics of turbulent ultra-lean premixed hydrogen flames. Our computational approach

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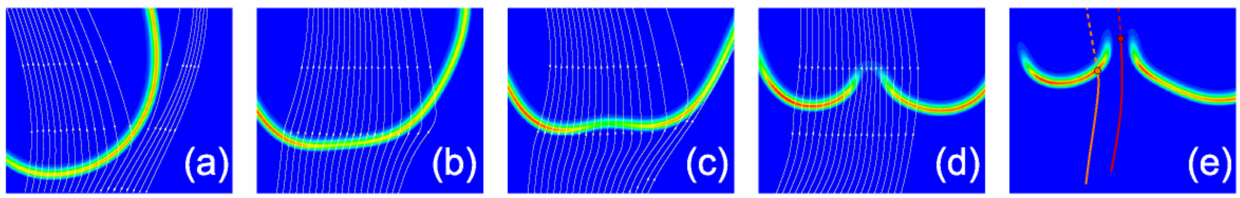

Figure 2: *Formation of an extinction pocket in an ultra-lean premixed hydrogen flame. The images depict regions 16mm wide at intervals of 3-5 ms from a 2D simulation. Overlaying lines in (a)-(d) indicate the instantaneous flow field, and in (e) indicate the Lagrangian trajectory during this sampling interval.*

exploits the natural separation of scale inherent in the system to incorporate the full range of spatial and temporal scales of laboratory experiments. A low Mach number approximation avoids integration of acoustic waves, which are fast but insignificant in open laboratory-scale flames. Adaptive mesh refinement focuses computational effort where needed to resolve thin reaction zones without using fine resolution away from the flame where it is not required. The adaptive low Mach number methodology reduces computational cost by approximately three orders of magnitude compared to traditional direct numerical simulation approaches.

In Figure 2, a time sequence of local fuel consumption from a simulation shows the formation of a local extinction pocket in a lean premixed turbulent hydrogen flame at conditions similar to the flame in Figure 1. As the flame is stretched and the burning intensity reduces, it recedes downstream locally. When the flame finally breaks (i.e. the consumption rate decreases markedly), the unburned fuel is redirected into channels that have strongly burning regions on the flanks. Once formed, these extinction channels persist robustly, disappearing only by merging with others, or through annihilation during large-scale folding of the flame surface.

The simulations allow study of the formation and long-time evolution of these extinction events, and the role they have in the generation of pollutants. In particular, we are beginning to understand the interplay of fluid strain, differential species transport and chemical kinetics near the flame surface. To obtain a quantitative understanding, we are developing new types of simulation diagnostics. One of these is based on a Lagrangian sampling of the solution along parcels of fluid as they pass through the flame. We can decompose the change in composition of each parcel into chemical and diffusive transport components, and relate them to the fluid environment and local flame geometry.

Ongoing work to unravel the coupling of differential species diffusion, turbulent fluctuations and detailed chemical kinetics is focused on characterizing these processes and their effects in laboratory-scale 3D flames, in close collaboration with experimental combustion scientists. The work includes the development and interpretation of new diagnostics, both from the simulation data and the laboratory experiment. By exploiting the natural scale separations of the problem, numerical simulations are enabling a new level of interaction between experimental and theoretical combustion scientists.

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