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Direct Numerical Simulations of Turbulent Lean Premixed Combustion

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Abstract. In recent years, due to the advent of high-performance computers and advanced numerical algorithms, direct numerical simulation (DNS) of combustion has emerged as a valuable computational research tool, in concert with experimentation. The role of DNS in delivering new scientific insight into turbulent combustion is illustrated using results from a recent 3D turbulent premixed flame simulation. To understand the influence of turbulence on the flame structure, a 3D fully-resolved DNS of a spatially-developing lean methane-air turbulent Bunsen flame was performed in the thin reaction zones regime. A reduced chemical model for methane-air chemistry consisting of 13 resolved species, 4 quasi-steady state species and 73 elementary reactions was developed specifically for the current simulation. The data is analyzed to study possible influences of turbulence on the flame thickness. The results show that the average flame thickness increases, in qualitative agreement with several experimental results.

1. Introduction

In many practical applications for power generation, such as stationary gas turbines, there has been a strong interest in achieving lean premixed combustion. The advantages of operating at lean mixture conditions are high thermal efficiency and low emissions of NOx due to lower flame temperatures. Since lean flames tend to be thicker and propagate more slowly, the small eddies of turbulence can enter the flame structure. Then, the small eddies can cause turbulent fluctuations of the temperature and reactant species ahead of the reaction zone, with the consequence that the scalar transport in and out of the reaction zone is enhanced. This regime is called the thin reaction zones (TRZ) regime [1].

There are limitations and uncertainities in the ability of models to describe premixed combustion in the TRZ regime. For example, it is not clear whether the flame dynamics in this regime is dominated by the entrainment of small eddies into the flame structure or the large scale flow straining which does not alter the flame structure. A lack of consensus on the effect of turbulence on flame structure in the TRZ regime is evident from the contradictory experimental results regarding the flame thickness. Several experimental studies in this regime have reported [2, 3] thicker flames, while others have reported thinner flames [4, 5]. Here we perform direct numerical simulation (DNS) to study the effects of turbulence on the flame structure and thickness in the TRZ regime.

In the past, due to the limited computational resources, DNS of turbulent combustion was limited to simple configurations such as periodic domains or all outflow configurations. Furthermore, complex chemistry simulations have been limited to two dimensions (2D) and three-dimensional (3D) simulations have been possible only with simple or tabulated chemistry. While these simplifications have been of great use in model development and validation in the past, they have lacked the realism of practical configurations. A spatially-developing flow configuration with at least one inflow is essential to represent laboratory-scale flames and to achieve statistical stationarity. Spatially developing flame simulations in 3D with detailed chemistry have been possible only recently due to the advances in computing power. Tanahashi *et al* [6] and Bell *et al* [7] have studied the propagation of hydrogen-air and methane-air flames, respectively, in 3D homogeneous turbulence at conditions relevant to the TRZ regime. Here, we have performed a fully-resolved DNS of a 3D spatially-developing lean methane-air premixed flame in the slot-burner Bunsen configuration with detailed chemistry. These simulations have been enabled by Office of Science leadership computing facilities at the National Center for Computational Science (NCCS).

2. Numerical Method

The simulations were performed using Sandia's massively parallel DNS code, S3D, which solves the full compressible reacting Navier-Stokes, total energy, species and mass continuity equations coupled with detailed chemistry. Time advancement is achieved through a six-stage, fourth-order explicit Runge-Kutta (R-K) method [8], spatial differencing is achieved through eighth-order finite differences with tenth-order explicit finite-difference filters on a structured, Cartesian grid [9], and Navier-Stokes Characteristic Boundary Conditions (NSCBC) [10, 11] were used to prescribe the boundary conditions. Recently, an improved characteristic boundary condition treatment [12] for compressible reacting flows with multi-dimensional and reaction effects has been developed under the SciDAC Terascale Simulations of Turbulent Combustion (TSTC) project. These improved boundary conditions will be used in future simulations to inject higher turbulence intensities at the inlet without numerical instability.

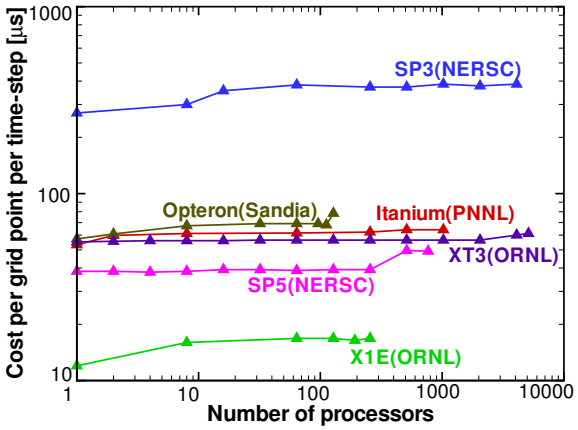

Figure 1. S3D cost of execution versus number of processors on several Office of Science computing platforms.

The equations are solved on a conventional structured Cartesian mesh, and scalable parallelism is achieved through MPI and a domain-decomposition strategy. Figure 1 shows the parallel speed-up of the code on several Office of Science platforms. In these tests the problem size per processor is fixed, and the total problem size is increased in proportion with the number of processors. It may be observed that the code scales very well on all platforms. On 5120 XT3 processors at NCCS(ORNL), 90% parallel efficiency is observed.

3. Problem Configuration

A planar-jet turbulent Bunsen flame configuration was used. Preheated methane-air mixture at 800K and $\phi = 0.7$ flows through a rectangular slot. The reactant jet is surrounded by a hot coflow whose composition and temperature are those of the complete combustion products of the main jet. While the configuration is chosen to be qualitatively similar to those used

in experiments [13], the jet size and velocity, mentioned below, are very different. At these conditions, the unstrained laminar flame properties computed using PREMIX [14] are: (i) flame speed, $S_{\rm L} = 1.8$ m/s (ii) thermal thickness based on maximum temperature gradient, $\delta_{\rm L}$=0.3mm.

The domain sizes in the streamwise (x), crosswise (y) and spanwise (z) directions, in terms of the slot width ($h = 1.2$mm), are $L_x \times L_y \times L_z = 12h \times 12h \times 3h$. A uniform grid spacing of 20μm was used in the x and z directions, while an algebraically stretched mesh was used in the y direction. The stretched mesh has a uniform spacing of 20μm in a 6mm wide region in the center and stretches outward with a rate of increase in grid spacing ($\Delta_{i+1}/\Delta_i - 1$) no more than 2%. The resultant mesh size was $N_x \times N_y \times N_z = 720 \times 400 \times 180$.

A hyperbolic tangent function was used to obtain a smooth variation between the unburned jet flow and the burned coflow at the inflow, where the width of the transition was equal to the laminar flame thickness. The presence of the surrounding hot coflow also serves to anchor the flame at the inlet. The species mass fractions and temperature at inlet were obtained from an unstrained laminar flame solution using a progress variable lookup. The velocity field at the inflow boundary was obtained by performing a separate temporally-developing simulation of a streamwise periodic flow. This secondary simulation was performed for a short period of time to allow sufficient development of the flow field and the resultant field was then frozen (in time) to obtain the inflow conditions for the main simulation using Taylor's hypothesis. At the jet inlet centerline, $\tilde{U} = 60$m/s, $u' = 18$m/s and the turbulence length scale was $l_{\rm t} = 0.15$mm. There is also generation of turbulence in the domain due to the shear instability between the jet and coflow. The velocity profiles at the inlet and the evolution of turbulence scales in the downstream direction are described in detail in Ref. [15]. The jet Reynolds number based on the centerline inlet velocity and slot width is $Re_{\rm jet} = 840$.

A reduced chemical mechanism for lean premixed methane-air flames was derived, specifically tailored to minimize temporal stiffness in DNS while maintaining accuracy. The reduction was accomplished through the sequential application of directed relation graph (DRG), sensitivity analysis and computational singular perturbation (CSP) [16] over the GRI-1.2 detailed mechanism. A notable aspect of the reduced mechanism is that the quasi-state species (QSS) concentrations were obtained through explicit analytical expressions without the need for expensive iterations. Consequently, overall convergence was obtained at a lower cost. Furthermore, eliminating the need for iterations facilitated good performance on vector computing platforms.

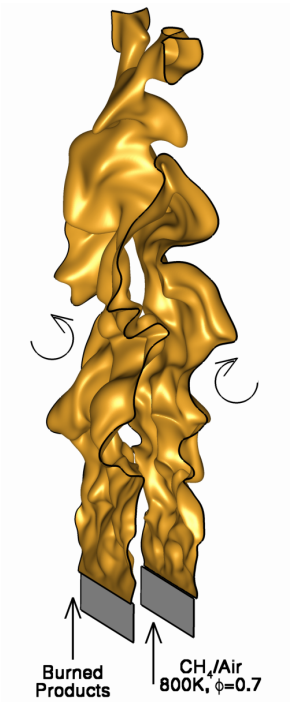

Figure 2. Flame surface denoted by the instantaneous iso-contour of c=0.65 at t=1$\tau_{\rm U}$.

4. Results and Discussion

Instantaneous Flame Structure

A reaction progress variable, c is defined based on the mass fraction of O_2. Here, we present the characteristics of the instantanenous flame front, identified as the iso-surface $c = 0.65$. Figure 2 shows the flame surface after one flow through time. The flame is initially planar near the inlet and shows considerable development with downstream distance. It is considerably wrinkled and the scale of wrinkling progressively gets larger. The shape of the flame is mostly convex towards the products and forms cusps towards the reactants, contrary to Huygens propagation. Evidently, turbulent straining has a stronger influence on the flame topology than self-propagation. Further downstream, the surface shows large scale roll-ups due to the

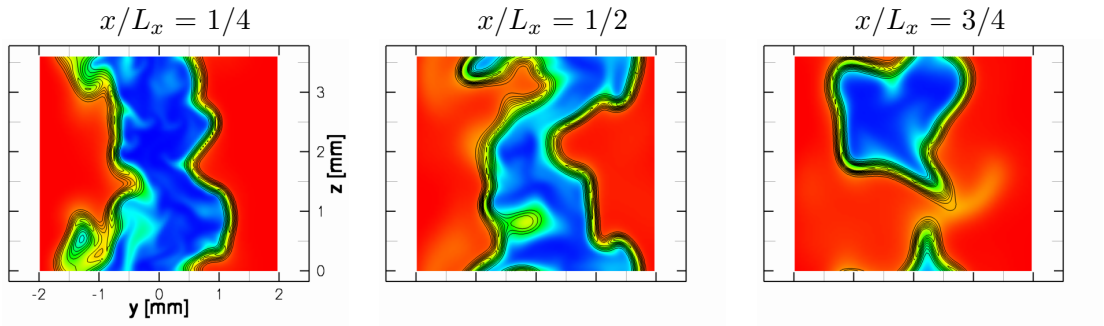

Figure 3. Instantaneous flame structure at different spatial locations and at time t=1τ_U. Color contours show the progress variable varying from 0 (blue) to 1 (red). Lines are the iso-contours of heat release rate.

presence of mean shear and mixing layer instability, leading to pinch off at the tip.

The instantaneous structure of the flame is also shown in Fig. 3, where the progress variable , c, is shown as color contours and heat release rate is shown as line contours. Figure 3 shows 2D slices of the flame surface in the y-z plane at different x locations, starting from the upstream location ($x/L_x = 1/4$) to the downstream location ($x/L_x = 3/4$). Initially there are two separate flame surfaces and they later interact and merge into a continuous surface at the far downstream location, which can be attributed both to fuel consumption at the core of the jet and to the pinch-off events at the flame tip. The flame structure near the unburned side is significantly disrupted as seen from the color contours. The heat release layer, especially on the burned side is relatively unperturbed which is evident from the parallelism of the line contours. This is due to the dissipation of turbulence resulting from heat release, thereby limiting the action of turbulent eddies to the unburned side of the flame.

Turbulent Flame Thickness

Here, we analyze the current simulation results to determine if, on average, the flame thickness increases or decreases relative to a laminar flame. The magnitude of progress variable gradient, $|\nabla c|$ yields a measure of the inverse flame thickness. Figure 4 shows the distribution of $|\nabla c|$ conditional on c. Also shown is the mean $|\nabla c|$ averaged over intervals of c compared with the unstrained laminar flame profile. Fig. 4 shows that, although there is some probability of

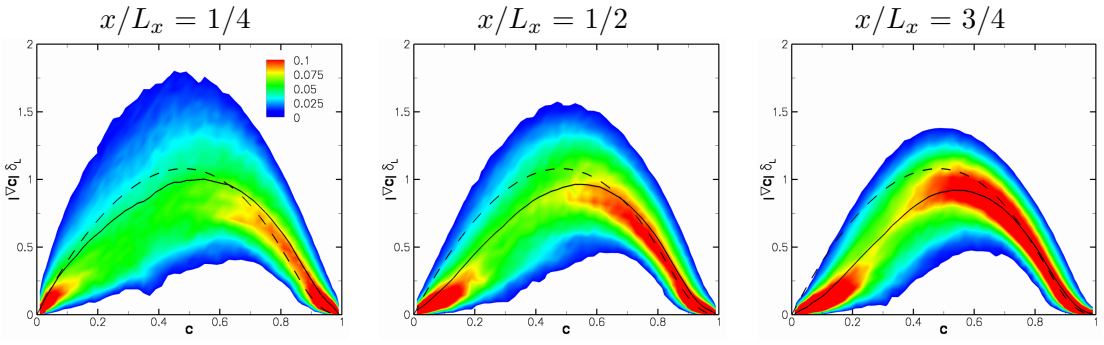

Figure 4. Color contours show the PDF of $|\nabla c|$ conditional on c using the standard rainbow scale varying from 0 (blue) to 0.1 (red). The conditional mean $|\nabla c|$ (solid line) is shown in comparison to the unstrained laminar flame profile (dashed line).

encountering a thinner flame, on average the flame thickness increases. It is seen that the mean $|\nabla c|$ is consistently lower than the laminar value and decreases with increasing x. At the '1/4'th location, a portion of the preheat layer closest to the fresh mixture has a mean gradient equal to the laminar flame thickness. However, at all other downstream locations, the average gradients in the preheat zone are clearly lower, pointing to a thickening of the flame. No significant deviation is seen for values of c close to unity, which corresponds to the oxidation layer. This again indicates that there is relatively less disruption of the oxidation layer by turbulence.

5. Conclusion

A spatially-developing 3D Bunsen flame was simulated using a computationally accurate and efficient detailed CH_4-air chemical mechanism derived specifically for this purpose. The simulation is performed long enough to achieve statistical stationarity. The results show that the average flame thickness increases, in qualitative agreement with several experimental results [2, 3]. In future, the data will be analyzed to study the detailed chemistry aspects of the simulation. In particular, the significance of simulations using realistic chemical model versus simplified chemistry will be studied. Furthermore, comparison and validation of different premixed combustion models in the TRZ regime is also planned.

Acknowledgments

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