Adaptive Low Mach Number Simulations of a Premixed Turbulent Laboratory Burner[1]

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Turbulent premixed combustion is a major active research topic in combustion science. A number of computational studies have focused on idealized configurations to aid in interpreting the dynamics of turbulent premixed flames observed in the laboratory, including one-dimensional strained flames, and two-dimensional vortex/flame interactions. More recently, researchers have begun to employ fully three-dimensional simulations, using varying levels of modelling sophistication to make up for the inevitable shortage in computational resources required for such an undertaking. Models are used to approximate turbulent sub-grid scale and inter-species transport, chemistry, and turbulence-chemistry interactions. These models take the form of unity Lewis number assumptions and LES or RANS type filtering on the fundamental transport equations. However, they introduce approximations that are difficult to justify; their validation is often through phenomenological matching to data and does not extend to a general class of configurations. Such shortcomings complicate the task of understanding and characterizing the basic interactions of fluid turbulence and combustion chemistry. Direct numerical simulations are an alternative approach for this task, attempting to simulate all relevant scales in the problem, thus minimizing the use of such heuristic models. But with the extrordinary expense of these multi-dimensional, multi-species time-dependent calculations, DNS is applied typically only over very small regions in physical space, representing idealizations of real combustion experiments with limited utility.

Low Mach number models fall, in some sense, between the filtered RANS/LES and DNS approaches, and are useful in the special (but practically ubiquitous) cases where acoustic information propagates at nearly infinite speeds with respect to the fluid advection. By filtering acoustic wave propagation from the underlying fluid model, numerical integration may proceed at time scales governed instead by the advective motion of the fluid. In tandem with robust discretization methods capable of accurately and stably representing the density contrasts associated with thermal expansion across flames with minimal resolution, low Mach number methods offer a uniquely efficient route to laboratory-scale combustion simulations. We have developed a low Mach number reacting flow simulation capability, which we apply to the study of a premixed turbulent laboratory flame. We combine the model with an adaptive grid technology so that we may perform simulations of full-scale experiments, including the cold-flow region inside the nozzle through the quasi-steady methane V-flame downstream. We do not use explicit models for a turbulent flame speed, or subgrid models for turbulent transport or chemistry turbulence interaction; we instead use a detailed 20-species, 84-reaction model for chemical kinetics and a mixture averaged model for differential diffusion. We present early simulation results, and current research aimed at characterizing the role of turbulence in the chemistry of an experimental rod-stabilized V-flame in the LBNL EETD combustion laboratory. Statistics gathered from the simulations and from the experiments are compared and discussed.

[1]Presented at: Western States Section of the Combustion Institute Fall Meeting, October 20-21, 2003.

Computational Model

We model the reacting flow in a laboratory burner as a mixture of perfect gases, ignoring Soret and Dufour effects, and radiative heat transfer, and assume a mixture-averaged model for differential species diffusion. The chemical kinetics are modeled using the DRM-19 methane mechanism. Our adaptive solution algorithm combines a symmetric operator-split coupling of chemistry and diffusion processes with a density-weighted approximate projection method for incorporating the velocity divergence constraint arising from the low Mach number formulation. Our approach to adaptive refinement is based on a block-structured hierarchical grid system composed of nested rectangular grid patches. The adaptive algorithm is second-order accurate in space and time, and discretely conserves species mass and enthalpy. The reader is referred to [1] for details of the low Mach number model and its numerical implementation and to [2] for previous applications of this methodology to the simulation of premixed turbulent flames.

Burner configuration

In the experiment, premixed air and methane at equivalence ratio $\phi = 0.7$ exit a 5 cm diameter circular nozzle with a nearly top-hat mean axial velocity profile of 3 m/s. Turbulence is introduced in the fuel stream by a perforated plate that partially obstructs the axial flow 9 cm below the nozzle exit. The observed integral scale length of the turbulence at the nozzle exit is ℓ_t ∼3.5 mm, as measured by pointwise LDV diagnostics. The fluctuation intensity is slightly anisotropic at u' ∼6.5% and ∼5% in the axial and radial directions respectively. A V-shaped flame is stabilized in the recirculation zone downstream of a 2 mm diameter rod spanning the width of the nozzle exit. The flame extends 20 cm or more downstream of the rod. Flow field and flame surface statistics are gathered from the experiment in a centered vertical plane normal to the rod up to 12 cm downstream of the nozzle exit.

We model the experimental domain in two stages, using an incompressible model for flow inside the nozzle, and a low Mach number reacting flow model for the flow downstream of the nozzle and into the flame. Results from the incompressible model provide a time-dependent inflow boundary condition through the nozzle to the reacting flow stage of the simulation. The fluid inside the nozzle is represented as a single-component, isothermal flow. Although the length of the nozzle is small enough that the observed exit flow has a tophat profile (very thin viscous boundary layer at the inside pipe wall), viscous effects are essential to the evolution of the turbulent fuel mixture. We assume a constant dynamic viscosity of $1.6{\cdot}10^{-5}$ m^2/s, corresponding to the value of the methane-air mix at 300 K. We make the significant simplifying assumption that the non-reacting fluid is reasonably approximated in Lagrangian coordinates, convecting at the mean nozzle flow rate, and is essentially unaffected by the side walls of the nozzle pipe. The simulation domain is a boundary-free triply-periodic cube, 5 cm on a side using a 256^3 grid. The flow is initialized with jets in one of the three directions, shaped to correspond to flow through the perforated turbulence screen. The reference frame of the domain is shifted to achieve a zero mean velocity. The flow is evolved for 0.03 seconds (the length of time it would take a fluid parcel travelling at the mean nozzle flow velocity to advect through the nozzle from the screen to the exit plane). At t =0.03

s, the computed integral scale length and turbulence intensity of the resulting simulated fuel agree with the measured quantities reported above, including the observed fluctuation anisotropy. By arguments similar to Taylor's hypothesis, the dimension parallel to the initial jets is interpreted as a time variable, and the data is fed into the time-dependent boundary of the low Mach number simulation to be described below. In accordance with an auxiliary simulation of the pipe flow using a compressible code equipped with an arbitrary geometry capability, the radial fluctuations of the inflow field were damped to zero at as $r \rightarrow$2.5 cm, corresponding to the location of the inside wall of the pipe. Axial fluctuations were increased by a factor of two at the pipe wall as well, for a more complete modelling of the auxiliary compressible solution. The Kolmogorov length scale for this flow is approximately 220 μm, and the turbulent Reynolds number is $Re_t = 39$.

The computational domain for the low Mach number stage of the simulation is a cube, 12 cm on a side, with the nozzle exit centered on the lower face. The sides of this domain are approximated as slip walls and the top is an outflow boundary. The fuel stream inflow profile is formed as the superposition of a mean flow at 3 m/s, and the turbulent fluctuations from the incompressible computation stage. We specify an air coflow of 1.5 m/s into the bottom of the domain outside the nozzle to control the shear layers that form around the outside of the fuel stream downstream of the inflow. In auxiliary 2D calculations, the flame surface shape was rather sensitive to the coflow velocity and domain size. We are currently assessing the extent to which this sensitivity carries over to three-dimensions, and how it is affected by the presence of significant turbulence in the fuel stream. Numerically, the flow in the low Mach number modelling region is initialized with room-temperature stagnant air through the domain, with a small hot region just above the rod. During evolution of the calculation, the heated air ignites a flame near the inlet, and the flame surface propagates downstream in the turbulent wake of the nozzle and rod. The resulting turbulent flame is evolved until it appears to be statistically stationary. The initial evolution is carried out with a 2-level adaptive grid hierarchy. A factor of two refinement from the base grid of 96^3 is added in regions of high vorticity and chemical activity (the flame front). After a quasi-steady flame is achieved, an additional grid refinement (another factor of two) was placed on the flame surface and in regions of high vorticity. This strategy resulted in approximately 12% of the domain being refined to the highest level. In separate calculations, evolution of the flame was continued for both the 2-level and 3-level cases. Except for the additional fine scale flame detail available in the 3-level solution, no significant variations appeared between the two runs after considerable evolution. The process was then repeated for an additional factor of two near the flame surface ($\Delta x_{eff} = 156.25 \mu m$), again with no significant deviations in the solution profiles. These resolution studies are a heuristic confirmation that the flame surface features of present interest are well-captured by our adaptive projection method, even at the rather coarse grid resolution of $\Delta x_{eff} = 625 \mu m$.

Observations

In Figure 1, we compare computed and experimentally observed instantaneous flame profiles. The image on the left is a grey-scale representation of the simulated methane mole fraction, taken in a vertical plane normal to the flame-holding rod at its center. The dark V-shaped region in the center indicates fuel depletion by combustion; the outer boundary is

perturbed by diffusion and convective interaction with the coflow stream. The corrugated surface of the flame indicates the level to which the turbulent inflow wrinkles the flame surface. The image on the right shows PIV data taken from an experiment with conditions similar to those of the computation. The premixed fuel is seeded with alumina particles that are illuminated by a vertical laser sheet. The darker V-shaped central region results from a decrease in fluid density, and a corresponding decrease in the density of flow markers as the reactants burn at the flame front. Clearly, the computations have reproduced qualitatively the experimentally observed flame shape and flame surface behavior for this case.

To construct statistical measures of the flame we define a progress variable $c = (\rho_u - \rho)/(\rho_u - \rho_b)$ where $\rho_{u,b}$ are the mass densities of the unburned and burned gas. The mean flame position then may be visualized as the mean location of a contour in c. We observe that the V-flame appears to be statistically invariant to the coordinate parallel to the rod in the range (± 1.5 cm), and is essentially symmetric about the center. Thus, we define

$$\bar{c}\,(x,z) = \int_{-1.5}^{+1.5} \int_{0}^{\Delta t} 0.5\,[c(-x,y,z,t_0+\tau) + c(x,y,z,t_0+\tau)]\,d\tau\,dy$$

where t_0 and Δt are large enough to eliminate the influence of early time transients and provide a good statistical mean. Based on the $\bar{c} = 0.5$ contour, we deduce that the computed turbulent flame angle is roughly 10 degrees. As discussed earlier, this angle is likely to be affected strongly by our assumptions on the coflow profile and domain size, and to a lesser extent on modeling simplifications such as the laminar flame speed of the chemical mechanism used in the model. The extent of influence of these and other factors will be the subject of ongoing investigations.

In Figure 2a, we overlay the $\bar{c} = 0.5$ (in red) contours and several representative instantaneous isosurface slices in planes normal to the rod at locations chosen randomly from the interval used to define $\bar{c}$. Similar information is presented from the corresponding experimental data in Figure 2b. Using such plots, experimentalists infer an effective flame area enhancement factor, i.e., ratio of areas of the actual flame surface to that of the mean flame. Early results suggest the computations predict an enhancement factor of 1.25, or a 25% increase in effective flame area due to turbulence.

In Figure 3, an isosurface of the temperature gradient ($= 10^6$ K/m) is used to visualize the flame surface in 3D. Note that in regions with significant reactions, this surface corresponds almost identically to the $\bar{c} = 0.5$ surface. However, the surface is "open" on the sides corresponding to where the gradient drops, indicating the absence of a flame (and corresponding to the flame surface observed visually in the laboratory). The $\bar{c} = 0.5$ surface is "closed" all the way around as it must be since the progress variable increases monotonically from 0 in the reactants to 1 in the products, regardless of whether a flame is present, and therefore provides a somewhat misleading picture of the reaction zone.

Conclusions

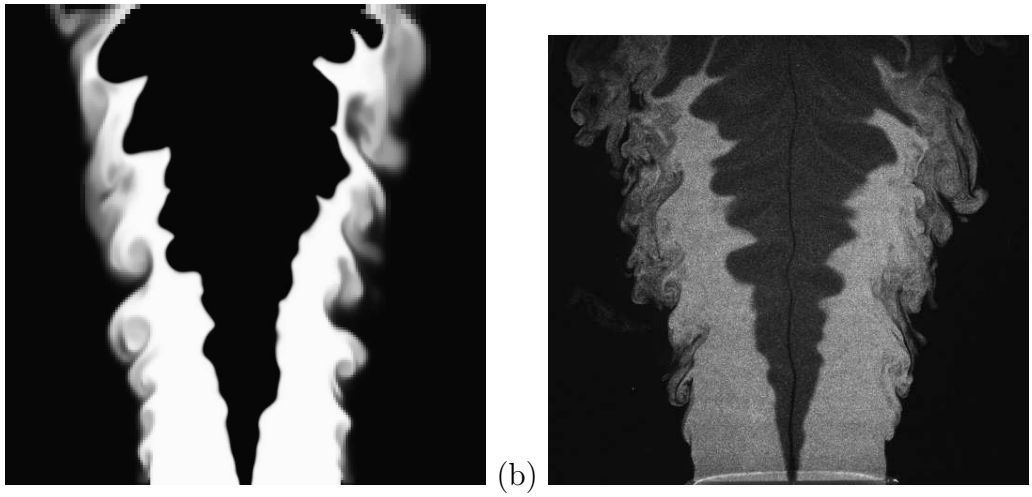
We have presented simulations of a laboratory-scale rod-stabilized turbulent V-flame burner without subgrid models for turbulence or turbulence/chemistry interactions. Initial comparisons of our results to experimentally measured flame statistics indicate that our methodology is sufficiently accurate to model this type of flame. Cursory refinement studies

confirm the expected convergence properties of our numerical algorithm, and reinforce the utility of such a method for exploring laboratory-scale experiments. We point out however that detailed studies of flame intermediates is not likely possible with the present resolution. For a flat laminar methane flame at ϕ =0.7, the reaction zone is approximately 170 μm thick. The finest grids used in this study were 156 μm, just barely small enough to discern the detailed flame structure. On the other hand, the thermal thickness, $\Delta T/(\nabla T)_{max}$, of this flame is approximately 600 μm, and is reasonably well approximated, despite being resolved by only 1 grid point in the coarsest 2-level simulation. The work suggests that with a sufficiently robust and well-behaved numerical algorithm, the required resolution may be adjusted to suit the study of interest.

References

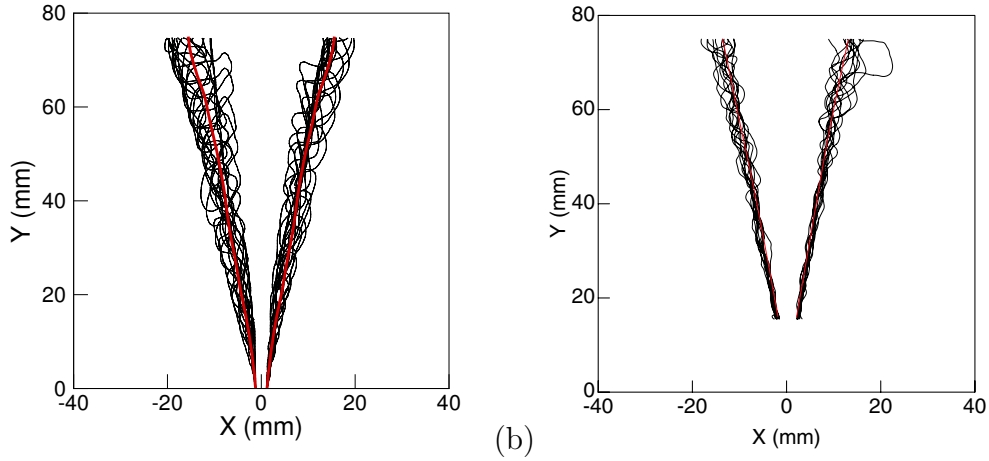
[1] Day, M. S. and Bell, J. B., *Combust. Theory Modelling*, 4(4):535–556 (2000).

[2] Bell, J. B., , Day, M. S., and Grcar, J. F., *Proc. Combust. Inst.*, 29 (2002).



(a) (b)

Figure 1. (a) Computed CH_4 mole fraction, (b) Illuminated particles seeded in fuel stream.



(a) (b)

Figure 2: Instantaneous flame edge in vertical plane, overlaid with computed mean, from (a) the simulation, and (b) experimental data

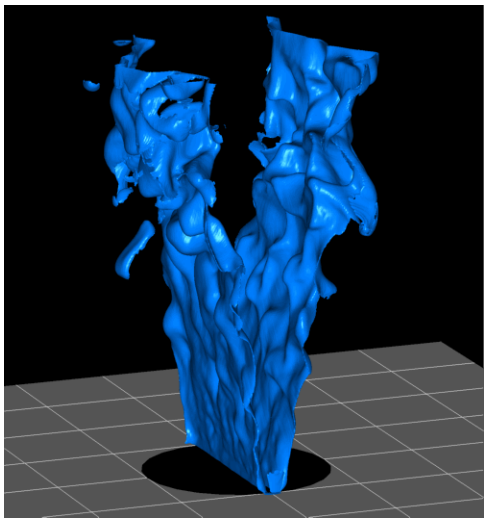


Figure 3: The flame surface, $\nabla T = 10^6$.