Numerical Control of 3D Turbulent Premixed Flame Simulations[1]

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Background

One of the well-known properties of turbulent, premixed flames is that their speed of propagtion is correlated to the intensity of the turbulence they encounter. A simple consequence is that these types of flames are inherently unstable. Given a source of turbulence, if the flame is propagating faster than the mean flow, it will drift upstream and encounter increased turbulent intensities that further accelerate the flame in the upstream direction. There will be an analogous deceleration if the flame speed is slower than the mean flow. To address this instability, experimental studies of premixed flames impose mean flow conditions faster than the turbulent flame speed and introduce some type of geometric or aerodynamic stabilization. Examples of these types of stabilized flames are V-flames, bluff-body flames, Bunsen flames, stagnation flames and swirl-stabilized flames. These types of flames are all the subject of active research in the experimental community (see the 29^{th} Proceedings of the Combustion Institute). Each of these configurations introduces its own particular features. For example, in stagnation flames there is a strong mean strain, in a bluff-body flame there is a larger recirculation zone, etc. The impact of the stabilization on flame properties introduces an additional complexity into the study of premixed turbulent combustion.

The inherent instability of turbulent, premixed flames also introduces problems for computational studies. One possibility is to attempt to include the flame stabilization mechanism in an overall reacting flow simulation. Thus approach has been pursued by Bell et al. [3] but the associated computational costs make this prohibitive for performing detailed parametric studies. A popular alternative configuration employed in direct numerical simulations (DNS) involves a doubly-periodic box domain with inlet and outflow boundaries in the direction of the mean flow. A 1D steady solution is used to initialize a flame and turbulent fluctuations are superimposed on the inlet flow. Such three-dimensional configurations were first studied by Trouvé and Poinsot [7] and by Zhang and Rutland [8] for simplified chemistry. More recently Tanahashi et al. [5, 6] have performed simulations of this type for turbulent, premixed hydrogen flames with detailed hydrogen chemistry. Bell et al. [1] performed a similar study for a turbulent methane flame. Unfortunately, due to the turbulent flame instabilities discussed above, the resulting flames are either accelerating or decelerating, and therefore encountering a time-varying turbulent intensity.

Bell et al. [2] introduce a feedback control algorithm for two-dimensional flows that automatically stabilizes a 2D "turbulent" flame in a configuration analogous to the DNS setting described above by dynamically adjusting the mean inflow velocity condition. This algorithm produces a statistically stationary, stable configuration where turbulence properties

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can be well characterized and detailed statistical information about the flame can be accumulated for analysis. In this paper, we extend that algorithm to 3D. We outline the basic simulation methodology and feedback control procedure. We then demonstrate the ability of the algorithm to stabilize such a premixed methane flame in three dimensions, and use the resulting flame to study a variety of flame-related combustion statistics.

Computational Approach

The simulations presented here are based on a low Mach number formulation. The methodology treats the fluid as a mixture of perfect gases. We use a mixture-averaged model for differential species diffusion and ignore Soret, Dufour and radiative transport processes. The chemical kinetics are evaluated using the GRI-Mech 3.0 without nitrogen chemistry. Transport and thermodynamic properties are taken from the associated databases. The basic discretization combines a symmetric operator-split coupling of chemistry and diffusion processes with a density-weighted approximate projection method to evolve the constrained advection. The resulting time-integration proceeds on the advective time scale. Diffusion and chemistry processes are treated time-implicitly. The basic integration scheme is embedded in a parallel adaptive mesh refinement algorithm framework based on a hierarchical system of rectangular grid patches. The complete integration algorithm is second-order accurate in space and time, and discretely conserves species mass and enthalpy. The reader is referred to [4] for details of the low Mach number model and its numerical implementation and to [1] for previous applications of this methodology to the simulation of premixed turbulent flames.

The basic geometry we consider is periodic in the x- and y-directions with inflow on the low-z face and outflow at the high-z face. The goal of the control algorithm is to automatically adjust the mean inflow velocity to fix the mean flame location on the grid. As an ansatz to developing the control algorithm, we assume there is an unknown turbulent flame speed, $\bar{s}_T$ that must be estimated as part of the algorithm. The actual instantaneous turbulent flame speed is not constant but will fluctate in time. If we view these fluctuations as a random forcing, we can model the flame location using the stochastic differential equation

$$dx = (v_{in}(t) - \bar{s}_T)dt + d\omega$$

where v_{in} is the mean inflow velocity and $d\omega$ represents fluctuations in the turbulent flame speed. The control problem can then be stated as: Given $x(0) = \alpha$, estimate s and find $v_{in}(t)$ so that $x(t) \to \beta$ where α and β are the initial and target flame locations, respectively.

Because the control velocity $v_{in}(t)$ determines the boundary condition for the low Mach number solver, we would like the control velocity to be relatively smooth in time. Consequently to suppress fluctuations in $v_{in}(t)$ resulting either from actual fluctuations in the turbulent flame speed or noise in its estimate, we introduce a time scale τ which is the target lag for reaching the desired state. We assume that τ is sufficiently large that the noise $d\omega$ has mean zero over the interval $[t, t+\tau]$. Then, given $x(t_0)$ and $v_{in}(t_0)$, we can integrate the ODE

$$\beta = x(t_0 + \tau) = x(t_0) + \int_{t_0}^{t_0+\tau} v_{in}(t_0) + (t - t_0)\Delta v - \bar{s}_T^{est} dt$$

and solve for Δv, the slope of the linear profile such that $\beta = x(t_0 + \tau)$. Here, the estimated speed, $\bar{s}_T^{est}$, is computed from the average change in fuel mass in the domain during some

number of previous time steps. (In practice, we have not found the algorithm to be sensitive to this estimate and have been able to use a single time step of data.)

Computational experiments on the stochastic ODE with zero mean, uniformly distributed fluctuations indicate that $\tau = O(10)\Delta t$ provides a smooth, responsive control. For the purposes of coupling to a flow solve we impose two additional constraints on the control. In particular, we require the that the control not change the velocity by more than 5% during a time step and that the control velocity not become negative. In practice, we observe long wavelength variations in the turbulent flame speed. Rather than trying to estimate a mean turbulent flame speed over a long time interval, the algorithm uses localized estimates so that we actually recover the smooth variation of s_T in time.

Preliminary Results

We consider a lean ($\phi = 0.55$) premixed methane flame as it interacts with turbulence in the inflowing fuel stream. At these conditions, the chemical mechanism predicts a laminar flame speed, $s_L = 7.62$ and a thermal thickness, $\delta_L^T = 1.31$ mm. The computational domain has dimensions $(15.2 \times 15.2 \times 30.4)\delta_L^T$, We specify inflow turbulence with integral scale $\ell_t = 1.85\ \delta_L^T$ and turbulent intensity, $u' = 2.04\ s_L$. Adaptive refinement based on the mass fraction of HCO and magnitude of vorticity are used to resolve in the inflow turbulence and maintain approximately 21 uniform grid cells across the thermal width of the flame.

We show in Figure 1 the flame location and control velocity as a function of simulation time, scaled to the turnover time of integral scale eddies, ℓ_t/u'. We set the target flame height to 0.5 cm for this example. This arbitrary location represents a balance between holding the flame near the inlet where the turbulent fluctuations have not undergone significant decay, while allowing enough space in the domain below the flame to accommodate surface excursions due to turbulent wrinkling. We initialized the solution with a 1D flame solution, and set the initial flame position lower than our target value. The initial transient apparent in Figure 1 indicates that the control quickly increases the fueling rate to shift the flame upward. As the target height is approached, a small overshoot is observed, and the inflow velocity is adjusted automatically to zero over a finite time interval. The control velocity then increases as the flame burns back to the desired location. Due to the flame surface wrinkling, the inlet velocity during the late-time evolution is controlled to a value somewhat higher than the laminar burning velocity. In Figure 2, we show a temperature isosurface corresponding to peak heat release. The surface is colored with CO mass fraction illustrating the chemical variability along the flame surface. In Figure 3 we show the fuel consumption at the peak and trough of the flame surface showing the expected correlation with fuel consumption and curvature. Quantitatively, these locations correspond to local flame speeds of 8.3 cm/s and 7.0 cm/s, respectively, corresponding to almost 20% variability in flame speed as a function of curvature.

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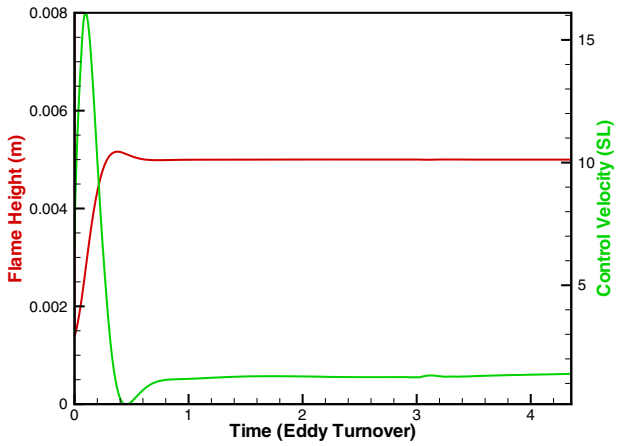

Figure 1: Flame location and control velocity.

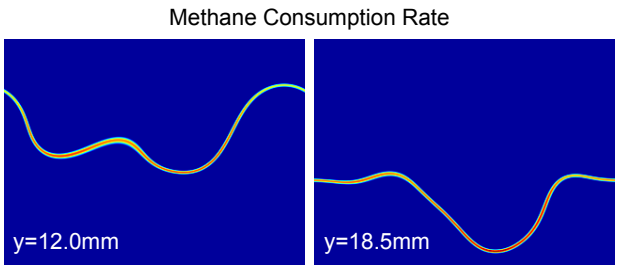

Figure 3: Vertical cross sections of fuel consumption.

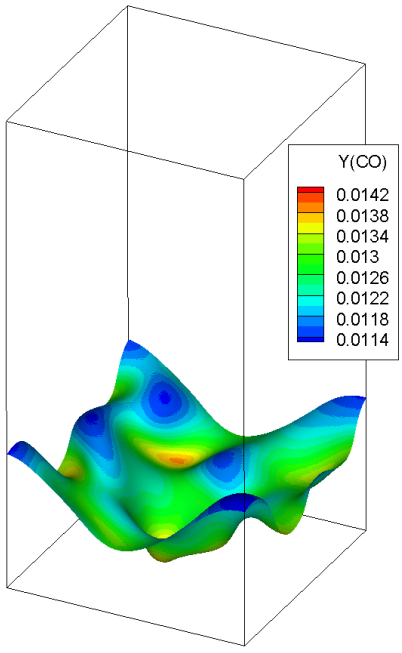

Figure 2: Temperature isosurface colored by CO mass fraction.