Tools for simulation of laboratory-scale premixed turbulent flames

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Abstract. We have entered a new era in turbulent combustion calculations, where we can now simulate a detailed laboratory-scale turbulent reacting flow with sufficient fidelity that the computed data may be expected to agree with experimental measurements. Moreover, flame simulations can be used to help interpret measured diagnostics, validate evolving flame theories, and generally allow exploration of the system in ways not previously available to experimentalists. In this paper, we will discuss our adaptive projection algorithm for low speed reacting flow that has helped make these types of simulations feasible, and two sets of new issues that are associated with application of this approach to simulating real flames. Using a recently computed flame simulation as an example, we will discuss issues concerning characterization of the experimental conditions and validation of the computed results. We also discuss recent developments in the analysis and interpretation of extremely large and complex reacting flow datasets, and a new approach to simulating premixed turbulent flames relevant to laboratory-scale combustion experiments—a feedback-controlled flame stabilization method.

1. Introduction
Using modern computational algorithms and high-performance computing hardware, it is now possible to use detailed numerical simulation to link experimental observations in turbulent premixed combustion with a fundamental understanding of the processes underlying flame/turbulence interaction. The range of scales for this problem is nevertheless quite large. While the thickness of a typical premixed flame is 10-100 microns, the flame surface wrinkling that plays a key role in turbulent burning processes is governed predominantly by the energy-bearing scales of the turbulence, which are typically over an order of magnitude larger. In addition, larger-scale flow features on the scale of the combustion device (10-100 cm) act to stabilize the flow. Fluid residence times in such devices can range from 10-1000 ms or more, while chemical reactions can occur on a scale of microseconds or less. Laminar flame speeds are typically 10-100 cm/s, while the speed of sound in hot product gases is over 1000 m/s. The multiphysics/multiscale character of premixed combustion simulation at the laboratory scale indeed poses major challenges to simulation.

A straightforward approach to this sort of simulation is to fully resolve all length and time scales present in the system, i.e. direct numerical simulation (DNS). Such a treatment would require computational grid-spacing on the order of parts of a reaction zone thickness, and time steps that resolve the stiffest chemical and acoustical processes in the system. Based on the given scales, a three-dimensional DNS simulation using traditional uniform-grid approaches...
would require more than $10^{12}$ grid cells and $10^6$ timesteps(!). And, as we shall see, such a simulation would be unnecessarily wasteful, since the regions with “interesting” detail are highly localized, and the observable fluid-dynamical timescales are considerably longer than those that limit the numerics. On the other hand, approaches such as RANS and LES developed for large-scale engineering simulations are also inappropriate. These approaches introduce models for the physical processes at subgrid scales, which is exactly the aspect of the problem we wish to explore. Rather, the problem requires a computational approach that is dynamically adaptive, carefully avoiding resolution of unnecessary detail. In this paper, we discuss recent and current applications of one such approach. We summarize important aspects of the algorithm, and discuss emerging issues associated with simulating laboratory experiments. Novel approaches are discussed both for setting up alternative simulations and for interrogating the massive datasets that result.

2. Low Mach Number Reacting Flow Model

A characteristic typical of many combustion applications, both experimental and commercial, is that the flame speed and associated fluid velocities ($U$) are much less than the speed of sound ($c$), hence the Mach number $M \equiv U/c \ll 1$. For a broad range of applications in this regime, sound waves have little influence on the flame and flow structures, yet constrain computational integration approaches. It is possible to derive a low Mach number model that analytically eliminates acoustic wave propagation while preserving the bulk compressibility effects due to thermal processes such as chemical reactions and thermal conduction [1, 2]. In the low Mach number formulation, the compressible flow equations are replaced by a constrained system similar in structure to the incompressible Navier-Stokes equations. Essentially, acoustic disturbances are instantaneously relaxed, so that acoustic temporal stiffness is replaced with a global elliptic coupling.

Our algorithm for integrating the low Mach number model [3] is a predictor-corrector integration procedure that involves a conservative advance of the velocity, enthalpy and species, initially using a lagged approximation to pressure. The intermediate velocity field that results is then decomposed using a density-weighted projection [4, 5] to extract the component satisfying the constraint due to the low Mach number approximation. The projection step involves the solution of a self-adjoint, variable coefficient elliptic equation. For the species conservation equations a splitting method is used that incorporates a stiff ODE integration technique to handle the disparate time scales associated with detailed kinetics. The overall fractional step scheme defines an integration procedure to advance the fluid evolution equations using a time step that is constrained by the fluid velocity rather than the acoustic wave speed. For typical combustion applications, this increases the maximum time step by one to two orders of magnitude.

An adaptive implementation [3, 6] of this low Mach number reacting flow integration procedure discussed here is based on the block-structured AMR originally developed for compressible flow [7–9]. In this approach, the regions to be refined are organized into rectangular patches, with several hundred to several thousand grid points per patch. One is thus able to use rectangular grid methods described above to advance the solution in time; furthermore, the overhead in managing the irregular data structures is amortized over relatively large amounts of floating-point work. Refinement is performed in time as well as in space, with each level of refinement using its own time step, subject to the constraint that the time step at a coarse level be an integral multiple of the time step at the next finer level. User-specified error estimation and refinement criteria are used to dynamically adjust the refinement as the computation proceeds. For typical combustion applications, refinement can be focused around the flame front, resulting in 1-2 orders of magnitude in savings when compared to a uniform fine grid of the same effective resolution.

The adaptive projection framework runs on distributed-memory parallel architectures using a
reusable software framework that handles data distribution and communication [10]. A dynamic load balancing algorithm accommodates the changing workload as regions of refinement are created and destroyed during the computation. For combustion applications the load-balancing problem is complicated by the heterogeneous workloads associated with chemical kinetics. In large-scale simulations on massively parallel compute hardware, the most intensive portions of the calculations are typically the variable-coefficient linear solves associated with the velocity projection, and the pointwise ODE evolutions associated with evolving the chemical reactions. The balance of the two depends on many factors, including problem size, processor count and chemical complexity.

3. Experimental Turbulent Premixed Flames
A taxonomy of interaction regimes [11] for turbulence and flame chemistry is illustrated in a turbulent flame chemistry regime diagram, Figure 1. In the “wrinkled flamelet” regime, turbulence wrinkles the flame surface, but has no appreciable affects on the combustion chemistry. In the “broken reaction zones” regime, the flame chemistry is distributed due to vigorous turbulent mixing. Most industrial/commercial applications of premixed combustion operate in the “corrugated flamelet” regime, where a broad range of turbulent eddies upstream of the flame will not only wrinkle the flame surface, but may significantly disrupt the thermal structure of flame itself.

We are currently investigating a number of laboratory experiments operating in the corrugated flamelet regime to understand flame dynamics and pollutant formation for commercial combustion applications. Representative flame surfaces are shown in Figure 2 for three example configurations, which can be categorized by the physical mechanism used to stabilize the flame in the laboratory. In the low-swirl burner configuration [12], the flame is stabilized in the flow divergence region above the nozzle created by a swirling component of flow localized to a thin outer layer in the fuel inlet pipe. The slot burner configuration [13] is stabilized using a pilot-flame system surrounding the central rectangular core of fuel. The V-flame [14] is stabilized using a thin metal rod spanning the inlet flow. Simulations of these flames requires the specification of considerable flow and geometry detail in order to reproduce observed flame dynamics.

3.1. Flame Simulations
We have performed detailed simulations of a rod-stabilized V-flame that validate our adaptive projection algorithm for a three-dimensional, time-dependent laboratory-scale turbulent flame configuration [15]. A photograph of the laboratory V-flame experiment appears as an inset in Figure 3. A methane/air mixture issues from circular nozzle. Turbulence is introduced into the fuel stream by a perforated plate mounted upstream of the nozzle exit. The flame is stabilized by a thin rod spanning the nozzle at its exit. The visible flame extends 15 cm or more downstream from the rod. A schematic of the computational domain is shown in Figure 3. Our approach to simulating the flame was to independently characterize the turbulence generation process using a combination of experimental measurements and auxiliary simulation. We then use this data as input for a reacting flow simulation in a cube, 12 cm on a side, with the nozzle exit centered
Figure 2. Laboratory-scale methane flame simulations illustrating three stabilization methods used in turbulent premixed combustion experiments: low-swirl stabilization, pilot-stabilized slot burner, and rod-stabilized V-flame.

on the lower face. The flame stabilization rod is modeled as a narrow no-flow strip at the nozzle exit. An air coflow into the bottom of the domain outside the nozzle provides a relatively crude approximation to the laboratory environment of the flame. The calculation incorporates the DRM-19 subset of the GRIMech-1.2 methane mechanism [16]. DRM-19 is a detailed mechanism containing 20 chemical species and 84 fundamental reactions. The solution is evolved with a 3-level AMR structure, where fine grid cells dynamically track the fluctuating flame surface. The analysis was based on 43.3 ms of simulated data, taken at 0.44 ms intervals after the flow reached a statistical equilibrium. The computation progressed approximately 38 µs per hour on 256 processors on the seaborne machine at NERSC An image of the instantaneous flame surface at the final simulation frame appears as the rightmost frame in Figure 2.

Figure 3 shows the mean axial ($\langle W \rangle$) and transverse ($\langle U \rangle$) velocity components in a vertical plane centered on the circular nozzle for the simulation and the experiment. The dashed lines superimposed on the plots indicate approximately the zone occupied by the time-dependent flame surface over time. Below each of the color plates, horizontal cuts of the averaged data show direct comparisons between the simulated and measured data at height intervals of 20 mm. Profiles are shown only where experimentally meaningful values were available. Away from the rod, the computed and experimental velocity data shows good qualitative agreement. The simulation captures with remarkable fidelity the major features of the experimental data, i.e. flame generated outward deflection in the unburned gases, inward flow convergence and a centerline flow acceleration in the burned gases.

A notable difference in the velocity fields is that the experimental measurements just above the nozzle exhibit a depression in axial velocity at the centerline not apparent in the simulation data, which conversely shows a localized acceleration there. In the experiment, the flow near the rod involves complex vortex shedding leading to a turbulent wake that is not represented accurately by the simplistic treatment of the rod boundary condition we have used in the computation. As a result, the simulated flame is anchored to the top of the rod, whereas in the experiment the flame is stabilized in the shear layer between the recirculation zone behind the rod and the
Figure 3. (a) Computational setup for V-flame calculation. Mean axial (b) and transverse (c) velocities in the simulation and the experiment with profiles of both at 6 elevations. Regions with poor experimental signal are omitted from the profiles. Photo inset and experimental data courtesy R. Cheng, I. Shepherd and M. Johnson, Environmental Energy Technologies Division, LBNL.

The other major issue that arises in these type of simulations is the ability of the chemical dynamics to accurately predict the flame properties. Although not presented in detail here, the computation predicts a flame angle that is too large and a flame brush that is too narrow. This discrepancy can potentially be attributed to numerics or boundary conditions; however, chemistry and transport are also possible causes. At the resolution used here, we match the laminar burning velocity of the best available mechanisms for methane combustion. However, an independent comparison with experimental data [18] shows that at the lean conditions considered here, the computed burning velocity overestimates experimentally
measured values by 15-20%. The errors observed in both in our computed flame angle and flame brush thickness are consistent with a numerical burning velocity that is too high.

4. Flame Stabilization
From the perspective of trying to understand and quantify the effect of local turbulence on the flame speed and how this behavior is modulated by flame chemistry, we have seen that fluid-mechanical stabilization mechanisms are problematic in that they introduce considerable complexity into both the simulation and analysis of the flame data. To compute a statistically stationary turbulent premixed flame with spatial and temporal scales relevant to the experiments, but without introducing a fluid-mechanical stabilization mechanism, we have developed a numerical stabilization procedure based on stochastic feedback control. We consider an idealized configuration with inflow and outflow boundaries in the direction of flame propagation and periodic boundary conditions transverse to the flame. The control algorithm then automatically adjusts the mean inflow velocity to dynamically stabilize the mean flame location on the grid.

Figure 4 illustrates the performance of our new control algorithm on a two-dimensional “turbulent” flame test. For this test we used a reduced 2-step reaction mechanism [19] for methane combustion, and inflowed a time-dependent velocity field with a spectrum characteristic of isotropic decaying turbulence. Note that in this regime, enhancement in fuel consumption due to turbulent surface area generation exhibits relative fluctuations that can approach 50%. This observation also underscores the difficulty in defining, and computationally simulating a “turbulent burning speed” on time scales comparable to the eddy turnover period of the turbulence.

One of our target problems has been two-dimensional simulations of methane flames in the corrugated flamelet regime. Three such simulations were performed [19] with the stochastic control methodology using the GRIMech-3.0 mechanism (53 species, 325 reactions). The cases, with stoichiometries \( \phi = 0.55, 0.75, 1.0 \), correspond to increasingly faster and thinner flames. Adaptive mesh refinement was used in all the simulations to maintain approximately 22 uniform grid cells across the thermal width of the flames throughout their evolution. Dynamic refinement for these simulations was based on the magnitude of vorticity and on a flame marker, CH\(_3\).

In Figure 5 we show the computed fuel consumption rate for each of the three cases in
small subregions of each of the domains. The most interesting feature of the data is how the correlation of fuel consumption with curvature changes with equivalence ratio for these flames in otherwise identical turbulence/chemistry interaction regimes. A dependence of local flame speed on curvature is expected from wrinkled flame theory (cf. Peters [11]). As observed experimentally [20], the $\phi = 0.75$ flame is less sensitive to curvature effects than the other two equivalence ratios. The correlation between fuel consumption and flame surface curvature is related to the so-called “Markstein number” used as a measure of the response of the flame to stretching effects. The data provided by our simulations enables a detailed study of the relationship between chemical kinetics and transport and the Markstein number, and is being used to develop improved “flamelet” models [21] in the context of a finite-width flame structure.

Modern flamelet models are based on parameterization of complex flame chemistry with a small number of fluid-dynamical quantities. A successful flamelet implementation will allow the chemical detail to be computed and tabulated in an auxiliary calculation for efficient look-up during a coupled fluid-dynamical simulation. However detailed simulations such as ours are required for the development and validation of such models.

The control methodology, and related integral flame analysis, discussed above for two-dimensional applications extends naturally to three dimensions. We are currently investigating three-dimensional controlled flames, using a range of fuels, for the purposes of exploring turbulent flame surface wrinkling phenomena related to advanced, low-emissions fuels. Because hydrogen molecules are considerably lighter than hydrocarbon fuels, they are susceptible to a classical thermo-diffusive instability wherein flame wrinkles are exacerbated by the flame’s response to curvature and strain. In Figure 6, we show planar laser-induced fluorescence (PLIF) measurements of the OH molecule in a premixed hydrogen flame surface taken from a low-swirl burner experiment. Experimentalists use OH to identify the flame position in order to quantify flame surface wrinkling characteristics in different fueling and turbulence scenarios. Below the experimental image, we show a snapshot of OH concentration from a 3D turbulent controlled hydrogen flame simulation in the same operating regime. The simulation not only reproduces the observed wrinkling phenomena, but the patterns of OH signals peaks are reproduced quite well. In the rightmost image,
an isosurface \( (T = 1200K) \) from the simulation, colored by the fuel consumption rate, confirms that the fuel consumption is dramatically reduced along the cusped ridges in the dynamic flame. In cases such as this, local extinction renders analysis of the experimental data difficult. With detailed simulations, experimentalists have a greatly increased range of data at their disposal for understanding and interpreting these processes.

5. Diagnostic Algorithms

Traditional data analysis for detailed combustion simulations has been limited primarily to graphical representations of species concentrations, augmented with reaction path analysis, lower dimensional sensitivity analysis and the construction of probability density functions to capture statistical relationships. As our ability to handle chemical complexity evolves, there is an increasing need to develop new mathematical analysis algorithms falling into three categories: automated approaches for traditional analyses, novel approaches to data analysis and tools to facilitate comparison to experiment. In the limited space remaining here, we will summarize some of the more interesting of tools we have developed, and example applications of the tools illustrating their use in a premixed turbulent flame setting.

5.1. Path diagrams

One of the tools we have developed automates reaction path analysis and provides an interface for representing reaction networks [22]. Reaction path analysis is an accounting of the exchange of material among species in a chemically reacting system, and a reaction path diagram is used to convey the results of a reaction path analysis. It is a directed graph whose nodes are the chemical species, and edges connect two species if a reaction moves material from one to the other. We have developed an automated approach, and graphical interface, to generate reaction path diagrams. The tool requires data from the numerically simulated flame, along with the kinetics database describing the chemical mechanism used for the simulation.

The basic form of a reaction path diagram provides a global snapshot of the chemical behavior of the system. One generalization of the standard path diagram is a conditional path diagram. In a conditional path diagram the integrals used to compute the edge weights are performed over a subdomain where a specific condition is satisfied, such as a specific spatial location or a specific band of temperatures. A conditional path diagram is used below to display the results of analyzing a premixed flame interaction with a two-dimensional vortex.

5.2. Stochastic particles

One of the difficulties with traditional data analysis paradigms for reacting flows is that they provide an instantaneous picture of the solution that makes it difficult to capture how the system arrived in its present state. To obtain a more direct picture of the system dynamics, we have developed a new diagnostic algorithm [23] based on the concept of tracking individual “atoms” through the simulation. For example, if one wanted to study the behavior of a methane flame, one could numerically “tag” carbon atoms in the methane and follow their evolution through the system. We note that this task is considerably more complex than the simple particle advection algorithms available in higher-end commercial data analysis software, in that the particles additionally diffuse and react in a manner that strongly depends on the properties of its host molecule, which itself changes as the system evolves. Our algorithm interrogates a simulated flow field by following “particles” that track atoms representing one of the elements in the chemical system as they move through the fluid by advection, diffusion and chemical reaction. Our approach is based on an operator splitting in which we first compute the deterministic advection of the particle. We then apply a lattice-based probabilistic algorithm to model diffusion where the probability of a diffusive jump is a function of the local diffusivity.
of the host molecule. The chemical reaction terms are modeled using a similar type of discrete time approximation to the underlying stochastic process.

To analyze a given flow situation, we seed a collection of particles representing atoms of interest and generate an ensemble of particle trajectories using the precomputed Eulerian solution of the time-dependent conservation equations. Analysis of the resulting trajectories then provides a characterization of the behavior of the system. For steady flames, there are direct analogs between stochastic particle diagnostics and traditional flame diagnostics. For example, for a steady flame, a tabulation of chemical transitions along particle paths is the same as the reaction path diagram computed using integrated reaction rates computed from the steady solution. Similarly, one can equate residence times for an atom within a specific molecule to the molar concentration profile of that molecule. These relationships were used to validate both the stochastic formulation and the stochastic integration algorithm. However, the formulation allows a more general exploration of time-dependent flows.

In Figure 7 we show a typical application of the stochastic particle analysis for time-dependent flows. Here, a two-dimensional configuration was used to reproduce an observed interaction of a vortex with a rich premixed laminar methane flame. In both the experiment and simulation, the concentration of CH at the flame drops significantly as a vortex passes through the flame surface. The stochastic particle diagnostic tool was key to determining that the approaching vortex induces a strong flow tangential to the leading edge of flame surface. This flow relocates the dominate sources of hydrogenous flame radicals, thereby shifting the fate of CH$_3$ reaction intermediates to favor destruction by recombination. This shift toward recombination ultimately decreases the production of CH. The reaction path diagrams in Figure 7 are conditioned on each of the two sets of the diagnostic particles, and provide a clear quantitative representation of the detailed chemical processes involved.

Conclusions
Using computational algorithms tailored specifically to the flow and reaction regimes encountered in turbulent premixed combustion experiments, we are now able to simulate laboratory-scale flames without relying on arbitrary parameterizations of underresolved physical processes. Statistics from the time-dependent solutions are validated directly with experimental data, to the extent that such data is available. Once validated, the computed flames can be used to
give experimentalists a more detailed picture of the processes occurring within the interaction of turbulence and flame chemistry. Moreover, since many experimental diagnostics extract lower-dimensional statistics (such as 2D PLIF and particle image velocimetry (PIV)), computed solutions may be used to validate experimental data interpretation procedures. Since the computations are carried out with detailed representations of chemical and transport processes, the enormous simulation datasets must then be probed with new data analysis techniques, such as our stochastic particles algorithm, to understand precisely how the fluid-dynamics and flame chemistry interact. Finally, these detailed studies may be used to develop and validate advanced models for reducing the complexity and computational effort in detailed engineering design of combustors, burners, etc. This unprecedented level of simulation detail is changing the way experimentalists and flame theorists approach their research, and is expanding the linkage between the two.

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