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Direct Numerical Simulation of Turbulent Counterflow Nonpremixed Flames

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Abstract. This paper presents our recent progress in terascale three-dimensional simulations of turbulent nonpremixed flames in the presence of a mean flow strain and fine water droplets. Under the ongoing university collaborative project supported by the DOE SciDAC Program [1] along with the INCITE 2007 Project [2], the study aims at bringing the state-of-the-art high-fidelity simulation capability to the next level by incorporating various advanced physical models for soot formation, radiative heat transfer, and lagrangian spray dynamics, to an unprecedented degree of detail in high-fidelity simulation application. The targeted science issue is fundamental characteristics of flame suppression by the complex interaction between turbulence, chemistry, radiation, and water spray. The high quality simulation data with full consideration of multi-physics processes will allow fundamental understanding of the key physical and chemical mechanisms in the flame quenching behavior. In this paper, recent efforts on numerical algorithms and model development toward the targeted terascale 3D simulations are discussed and some preliminary results are presented.

1. Introduction

In recent years, the availability of massively parallel terascale computers has launched a new direction in the study of three-dimensional laboratory-scale combustion problems using the direct numerical simulation (DNS) approach [3,4]. In particular, a 2005 INCITE project led by Chen and Hawkes [5] has demonstrated that, while costly, three-dimensional turbulent direct numerical simulations with detailed chemistry enable both turbulence dynamics and chemical reaction to be accurately represented concurrently, thus opening new realms of possibility in answering important science questions related to turbulence-chemistry interaction and its implication to turbulent combustion modeling. More recently, three-dimensional DNS has also been applied to studying turbulent premixed flames [6,7]. Encouraged by these accomplishments, the proposed project is targeted to extend the high-fidelity DNS capability even further by incorporating multi-physics issues of turbulent flame quenching by water spray and radiation. The major tasks under this project involve implementation of advanced physical models, such as radiation, soot, and spray, into the structured-grid, high-order, non-dissipative reacting flow solver, thereby providing a computational diagnostic tool for spray dynamics, combustion, and pollutant formation processes that can impact the development of high-performance, low-emission combustion devices.

The study of spray-flame interaction has strong scientific and practical relevance, especially in fire suppression technology. Newer designs for water-based fire suppression systems are based on water mist systems [8]. While the conventional sprinkler systems achieve fire suppression by *fuel cooling* and by *flame spread inhibition*, water mist systems achieve suppression by *flame cooling* and have the potential of improved efficiency (reduced water demand) and performance (possible circulation around obstructions and shielded areas). Despite a growing interest in water mist systems, however, a fundamental understanding of the basic physical mechanisms that lead to fire suppression by fine water droplets is still lacking. Key relevant issues include: the injection and atomization processes, and overall early liquid water spray dynamics in the vicinity of the injector; the subsequent turbulent dispersion of the water droplets in the fire room and the probability of their transport to the flame location; and finally the interaction of evaporating water droplets with the turbulent flame, and the resulting decrease in combustion intensity and possible partial/total flame quenching. The high fidelity DNS is well suited to provide valuable information to address these issues.

This paper presents an overview of our recent accomplishments toward the terascale 3D simulations. First, some highlights on our recent study of the soot dynamics in turbulent nonpremixed counterflow flames are briefly summarized. Recent advancement in the development and implementation of the spray model in DNS is then described. Finally, some preliminary results on the interaction of water droplets and turbulent counterflow flames are presented.

2. Transient Soot Dynamics in Turbulent Nonpremixed Flames

The improved characteristic boundary conditions for compressible reacting Navier-Stokes equation solvers [9,10] enabled robust and accurate simulations of the counterflow turbulent nonpremixed flames. The new DNS capability has been applied to investigate the transient dynamics of soot formation processes in ethylene-air flames with a semi-empirical soot model [11,12] and optically-thick gas radiation model based on the discrete ordinate method [13]. In our recent study [14], the effects of different turbulent intensities on soot characteristics were examined.

Figure 1 shows instantaneous images of the soot volume fraction contours for the three different parametric cases considered. It was found that the most important parameter is the ratio of the integral eddy scale to the flame thickness (L_{11}/l_f). For a smaller ratio (Figure 1(a)), turbulent eddies penetrate into the flame structure, thereby spreading out the soot distribution more widely with a larger level of scatter. As the ratio increases to a larger value (Figure 1(c)), the effect of turbulence is primarily to suppress the soot formation with a reduced scatter in the data.

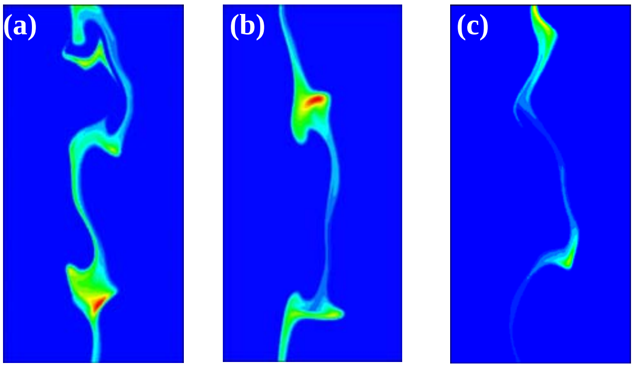

Figure 1. Instantaneous images of soot volume fraction in counterflow turbulent nonpremixed flames: (a) L_{11}/l_f = 0.58, (b) L_{11}/l_f = 1.16, (c) L_{11}/l_f = 1.58.

Detailed analysis of the data revealed that turbulence affects soot formation through three distinct paths depending on the local scalar dissipation rate and the rate of soot formation reaction: (a) low mixing and high reaction rates yielding a significant level of soot enhancement, (b) high mixing rate from large tangential strain rate leading to a reduction in soot formation, and (c) strong convective motion transporting high level of soot into low temperature and fuel-rich regions. As an overall consequence, turbulence has two competing effects on soot formation: enhancement by increased flame volume and reduction by rapid transport of soot pockets out of the high temperature regions. Since the increased turbulence intensity results in reduced Kolmogorov eddy scale, it is expected that the overall soot yield increases first due to the flame volume generation and then drops down as the effect of turbulent dissipation starts to dominate. The DNS results demonstrate that detailed information on the local and transient flow-chemistry interaction is essential in accurate prediction of soot formation characteristics in turbulent combustion.

3. Improved Spray Models and Application to Diesel Engines

One of the important aspects in the present project is the new capability of describing multiphase flow characteristics in high-fidelity simulations. The interactions between evaporating liquid droplets and a carrier gas-phase fluid has long been a significant modeling challenge. Compared to the DNS simulation of particle-laden flows, the application of DNS to evaporating liquid sprays at higher speed has only recently been addressed. Wang and Rutland [15,16] performed a systematic DNS study on the ignition process of an n-heptane fuel spray in a turbulent field using a detailed chemistry mechanism. In the current implementation of the spray model, a Lagrangian particle approach is coupled with the Eulerian solver for the gas-phase transport. The individual droplets are assumed to be spherical with constant density, and droplet interactions are neglected because the droplet sizes considered are small (less than 100μm).

In a recent study [17], we have investigated the effects of various parameters on the lift-off length of the diffusion flame established in the n-heptane spray jet into quiescent air. The objective was to validate the postulates on ignition and combustion behavior occurring in a diesel engine. In particular, the region in the immediate downstream of the spray tip has been studied in detail. Figure 2 shows two instantaneous images of the heat release rate for an n-heptane jet simulated in a realistic diesel engine conditions. At an early phase of ignition (0.6 ms), the ignition region surrounds the jet periphery. At a later time (2.7 ms), a fuel-rich premixed combustion is observed in further downstream of the jet. It was also found that the local equivalence ratio near the spray tip ranges between 2 and 4.5. All these results are found to be consistent with the experimental observations and the schematic diesel spray combustion model proposed by Dec [18].

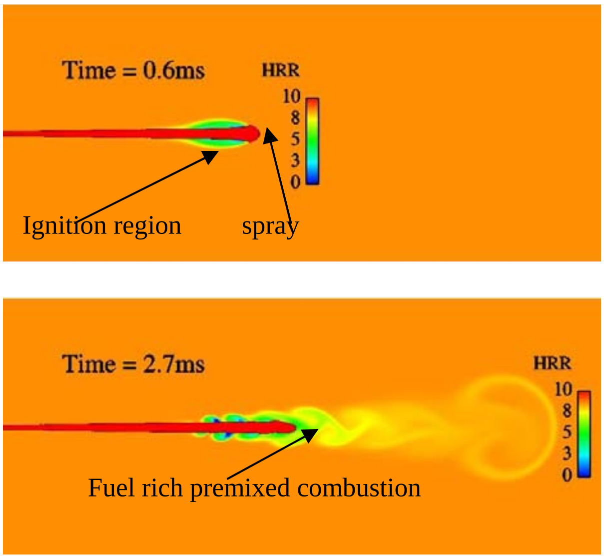

Figure 2. DNS simulation results for the heat release rate isocontours in a 200m/s n-heptane jet with droplet initial size of 20μm after 0.6ms (top) and 2.7ms (bottom).

4. Interaction of Turbulent Nonpremixed Flames and Water Spray

With the developed physical models, we have conducted some preliminary simulations of two-dimensional turbulent counterflow nonpremixed flames. The baseline case without spray is compared against the simulation with a water spray injection. Pure ethylene and air were injected at the two opposing inflow boundaries at the mean velocity of 78 cm/s. Turbulent eddies generated at the intensity of 1.5 m/s and with the integral scale size of 0.86 cm were injected at both inflow boundaries. After 2 ms of the baseline case simulation, the water spray was injected at 0.3 cm from the centerline of the domain at 50 m/s. The initial water droplet diameter was 20 μm and temperature was at 300K.

Figure 3 shows instantaneous images of vorticity, temperature, and heat release rate isocontours for the two cases - without and with the water spray injection. After 4 ms from the initial condition, the turbulent eddies injected through the inflow boundaries are fully convected into the domain and interact with the initially planar flame surface. The temperature and heat release isocontours for the baseline case (upper row) indicate that turbulence is affecting the local flame intensities, although partial extinction was not observed at this specific time. In contrast, figures in the lower row exhibit significant flame weakening by the effect of the spray jet.

In this preliminary simulation, a small droplet size and large injection velocity were chosen for computational efficiency. In a practical system, a larger droplet size at smaller injection velocity is expected for effective global flame quenching [19]. Further simulations will be undertaken in order to investigate the effect of various spray parameters on the flame extinction behavior.

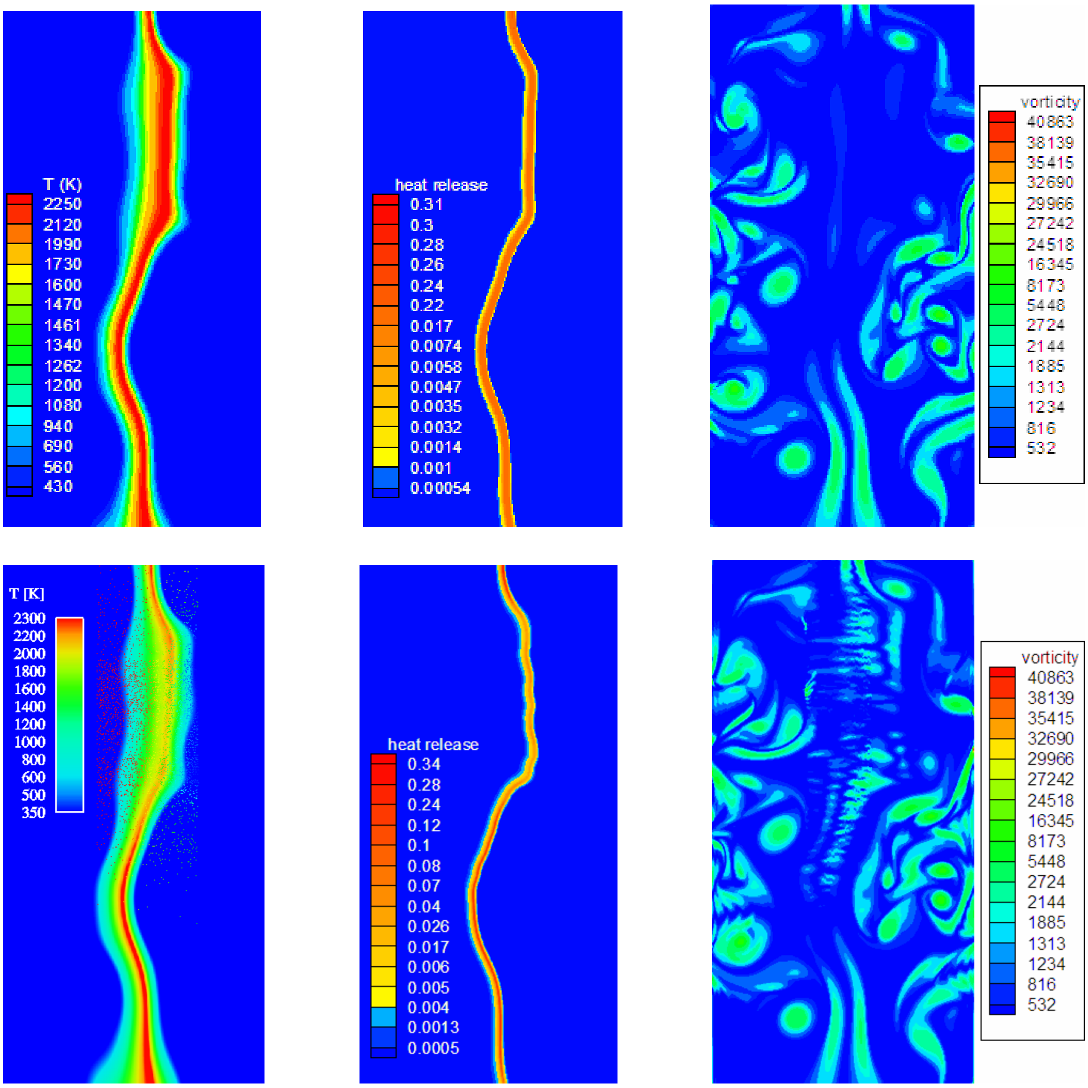

Figure 3. Isocontours of temperature, heat release rate, and vorticity for two-dimensional turbulent counterflow nonpremixed flames after 4 ms from the initial injection of turbulence. The upper row represents the solution fields without spray injection; the lower row shows the simulation results with spray injection after 2 ms from turbulent starting field.

5. Future Work

We have successfully developed and tested a simulation capability for turbulent nonpremixed flames in a counterflow configuration with advanced radiation, soot, and spray models. During the remainder of 2007, terascale three-dimensional simulations will be conducted as part of the SciDAC and INCITE programs. The simulation data will provide accurate information about local and temporal behavior of wrinkled nonpremixed flames subjected to turbulent strain and spray cooling, leading to intermittent extinction and reignition phenomena. The massive amount of data will be analyzed through high performance visualization and postprocessing techniques to provide a quantitative description of flame suppression by spray, in contrast to conventional stretch-induced turbulent flame extinction.

The SciDAC program provides excellent opportunities for interdisciplinary collaboration. For example, we are currently seeking and establishing collaborators with expertise on interactive distributed multi-variate visualization, effective feature-tracking for automatic detection of important observables, and automated reduction of chemistry-induced stiffness through elimination of fast time scales. More challenges need to be overcome in our efforts towards petascale simulations of turbulent combustion at practical laboratory scales.

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