High-fidelity simulations for clean and efficient combustion of alternative fuels

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Abstract. The monolithic nature of transportation technologies offers opportunities for significant improvements in efficiency of 25–50% through strategic technical investments in both advanced fuels and new low-temperature engine concepts. The application of direct numerical simulation (DNS) provides a way to study fundamental issues related to small-scale combustion processes in well-defined canonical configurations, whereas the application of large eddy simulation (LES) provides a formal treatment of the full range of time and length scales that exist in turbulent reacting flows, and thus provides a direct link to experimental studies of relevant combustion devices. In the present study, through DOE INCITE and Oak Ridge National Laboratory 250 Tflop Transition-to-Operations grants in 2008, DNS is performed to understand how a lifted autoignitive flame is stabilized, and LES is performed to understand the high-pressure injection and mixing processes in internal combustion engines. Understanding of these and other fundamental issues is needed to develop robust and reliable ignition and combustion models for the combustion regimes observed under low-temperature combustion engine environments using alternative fuels.

1. DNS of an autoigniting, turbulent-lifted ethylene/air jet flame
In many modern combustion systems such as diesel engines or direct injection stratified gasoline engines and gas turbines, fuel is injected into an environment of hot gases such that a flame may be stabilized through the recirculation of hot air and combustion products. Under such conditions, this process leads to a turbulent lifted flame, and the hot environment supports autoignition as a possible mechanism contributing to the stabilization of the flame base. In addition to autoignition, flame propagation and the role of coherent eddies have been considered as possible mechanisms for stabilization of the lifted flame [1]. In previous 3-D direct numerical simulation (DNS) study of an autoigniting, turbulent-lifted hydrogen/air jet flame, it was found that the lifted flame stabilizes primarily by autoignition that occurs in fuel-lean, hot mixtures in regions of low scalar dissipation (mixing rate) rate [1]. The present DNS study explores the stabilization mechanism for a hydrocarbon fuel with more complex ignition kinetics. In particular, a turbulent lifted ethylene/air jet flame in an autoignitive heated coflow is simulated, and the stabilization mechanism and flame structure are determined. Future DNS studies will examine the effects of renewable fuels (e.g., ethanol and biofuels) on flame stabilization, extinction and reignition, and stratified flame propagation.

An ethylene-air lifted flame in a spatially evolving slot-burner configuration was simulated on the Cray XT system, called Jaguar, at the National Center for Computational Sciences (NCCS).
Jaguar was recently upgraded with quad-core AMD OpteronTM processors, which raised the peak performance of the system from 119 teraflops to 260 teraflops. Prior to the upgrade, Jaguar consisted of 11,508 XT4 nodes each containing a 2.6 GHz dual-core AMD Opteron processor. After the upgrade, Jaguar consists of 7,832 XT4 compute nodes each containing a 2.1 GHz quad-core AMD Opteron processor. More important, while the dual-core Opteron processor was, theoretically, able to perform two floating point operations per clock cycle, the quad-core Opteron processor is able to perform four operations. The factor of 2 improvement in performance is due to an increase in the SSE execution width from 64-bit to 128-bit in the new quad-core processor. Vectorization and generation of SSE-instructions are essential to take advantage of the capabilities of the new quad-core processor.

The performance of the Sandia DNS code, S3D, with a detailed ethylene-air mechanism was evaluated using a pressure-wave test, where the propagation of a small amplitude pressure wave through the domain is computed for a short period of time. The fixed problem size contained $30^3$ grid points per MPI-thread. Earlier performance studies have shown that S3D can scale up to the entire size of the system on various Office of Science platforms, and show near-ideal weak scaling performance. For brevity, only the single socket performance data is presented here, with a note that the near-ideal weak scaling behavior was observed across the entire system nodes. Table 1 shows a comparison of the time taken to compute the ethylene-air problem on the old XT with 2.6 GHz dual core Opteron and the newer XT with 2.1 GHz quad-core Opteron. For comparison, the table contains performance data for an undersubscribed processor with fewer threads than the number of cores. Practical S3D simulations use all cores in a socket. The initial port to quad-core processor showed a decrease in performance: it took 503 seconds on the quad-core in comparison to 465 seconds on dual-core. Part of this decrease is attributable to the lower clock speed. Clearly, however, vectorization was not as aggressive as desirable.

Special effort was devoted to rewriting the chemistry evaluation routine, which was consuming roughly 60% of the overall run time. With assistance from the Cray Supercomputing Center for Excellence, the routine was rewritten to operate on data at multiple grid points using array syntax to facilitate SSE instruction generation. A larger fraction of the floating point operations are performed through SSE instructions as a result of the code improvement. A decrease in run time of roughly 20% was achieved, and the computation took less time (422 s) on the quad-core processor. The production simulation was then performed using 30,000 Opteron cores on Jaguar consuming 4.5 million CPU-hrs and generated half a terabyte of data every hour.

### Table 1

| Problem Size | Mpi-mode | Dual-core | Quad-core (initial) | Quad-core (vectorized) |
|--------------|----------|-----------|---------------------|------------------------|
| $30 \times 30 \times 30$ | -n 1 -N 1 | 404 | 415 | 333 |
| $60 \times 30 \times 30$ | -n 2 -N 2 | 465 | 430 | 349 |
| $60 \times 60 \times 30$ | -n 4 -N 4 | - | 503 | 422 |

The spatially developing turbulent lifted jet flame simulation was performed in a 3-D slot-burner configuration. Fuel issues from a central jet, which consists of 18% ethylene and 82% nitrogen by volume at an inlet temperature of $T_j = 550K$. The central jet is surrounded on either side by co-flowing heated air streams at $T_c = 1,550K$ and atmospheric pressure. The fuel jet and coflow velocities are specified as $U_j = 204 m/s$ and $U_c = 20 m/s$, and the fuel jet width, H, is 2 mm such that the jet Reynolds number, $Re_j = HU_j$, is approximately 10,000. The computational domain is $15H \times 20H \times 3H$ in the streamwise, x, transverse, y, and spanwise, z, directions with...
Figure 1. From Left: $Y_{HO_2}$, $Y_{CH_2O}$, and scalar dissipation rate in a lifted ethylene-air jet flame at Re=10,000.

2025 × 1600 × 400 grids for a total of 1.3 billion grids. A uniform grid spacing of 15 microns is used in the x- and z-directions, while an algebraically stretched mesh is used in the y-direction. The compressible Navier-Stokes, species continuity, and total energy equations were solved by using S3D with a fourth-order Runge-Kutta method for time integration and an eighth-order central differencing scheme for spatial discretization. We adopted a reduced ethylene/air kinetic mechanism which consists of 22 species and 18 global reaction steps (T. Lu and C. K. Law, private communication, 2007). Nonreflecting inflow/outflow boundary conditions [2] were used in the x- and y-directions and periodic boundary conditions were applied in the homogeneous z-direction.

Figure 1 shows volume rendering of hydroperoxy radical (ignition marker) and formaldehyde mass fractions and scalar dissipation rate (local mixing rate) fields. Downstream of the high scalar dissipation region, temperature starts to increase at $x/H = 6$, following an increase in the heat release rate. Global characteristics of the lifted flame represented by the Favre mean temperature and heat release rate show that, unlike the hydrogen/air lifted jet flame [1], the mean heat release rate starts to increase in the middle of the shear layer. This is attributed not only to the large stoichiometric mixture fraction of the present flame relative to the hydrogen flame but also to differences in the ignition kinetics/transport coupling in the ethylene/air jet flame.

The stabilization mechanism of the present ethylene/air lifted jet flame is further investigated by tracking Lagrangian fluid particles. Tracer particle methods are commonly used to gain fundamental understanding of intermittent flow and flame physics [3]. The particles provide the time history of the turbulence and mixing conditions that a given fluid parcel undergoes while being advected through the domain. In particular, it provides the temporal trajectory of a given localized ignition site as it traverses oncoming turbulence intermittency, thus providing valuable lagrangian velocity-scalar statistics for the validation of models predicting lift-off heights in autoignitive partially-premixed turbulent jet flames.

2. LES of direct-injection processes in internal combustion engines

Direct injection (DI) is a promising option for modern internal-combustion (IC) engines. In conventional diesel and homogeneous charge compression ignition (HCCI) applications, DI lowers soot and NO$_x$ production and improves fuel economy. In hydrogen-fueled engines, DI provides the appropriate energy density required for high efficiency and low NO$_x$. In order to realize the full benefit of DI, however, the effect of various injection parameters, such as injection timing, duration, pressure, and dilution, must be investigated and optimized under a range of operating conditions. As part of our 2008 INCITE grant, Oefelein has developed a model for high-fidelity
calculations of DI processes using the large eddy simulation (LES) technique and coupled this with an advanced property evaluation scheme designed to handle high-pressure phenomena. The theoretical-numerical framework enables both the canonical cases described here and in-cylinder calculations that will be performed subsequently. Here we focus on high-pressure multi-port gas injectors designed for application in hydrogen-fueled IC-engines. To investigate issues related to high-pressure gas injection processes, we have developed a general model framework that combines a detailed property evaluation scheme for arbitrary gas-liquid hydrocarbon mixtures with the LES technique [4]. In LES, the large energy-containing scales of fluid motion are solved on a computational grid. The small (more universal) subgrid-scale interactions are modeled. This approach allows time-accurate predictions of turbulent flows at extremely high Reynolds numbers. As a step toward systematic validation, we have considered a series of cases using the experimental data acquired by Petersen and Ghandhi [5] for validation. Following is a brief description of simulations enabled by the current INCITE grant.

High-pressure, multiport hydrogen injector studies were conducted in an optically accessible chamber by Petersen and Ghandhi [5]. Single, three, seven, nine, and thirteen port injectors were considered. Jet flow patterns were visualized by using a Schlieren technique. The images were processed to determine the penetration length and angle. The pressure history during injection was also measured to determine the mass flow rate of the injected gas. Injection pressure, chamber density, and chamber gas composition were varied to isolate the effects of pressure, density, and compressibility. As part of our effort to validate the fully coupled theoretical-numerical framework, we have performed a series of high-fidelity LES calculations of the three hole injector. We focus on three cases, where hydrogen is injected into nitrogen at 10.4 MPa, with chamber pressures fixed at atmospheric, 340 kPa and 720 kPa. This set of conditions places the system in the supercritical regime.

A representative result is given in figure 2, which shows the level of qualitative agreement obtained between experimentally observed and simulated results for the case when the chamber pressure is 340 kMPa. On the left is the instantaneous shadowgraph from the experiment. On the right is instantaneous iso-contours of density from the LES solution at the same instant in time. Blue represents the density of the pure hydrogen stream (0.273 kg/m$^3$), red the density of pure nitrogen (3.80 kg/m$^3$) and yellow an intermediate value (2.04 kg/m$^3$). Similar agreement has been obtained for all cases. Comparisons between the shadowgraph data and corresponding LES suggest that the fine-scale turbulent structure, which dominates the spatial evolution of the flow, can be reproduced quite accurately in the simulations. This is a crucial requirement for developing accurate predictive models and provides a way to perform detailed analysis of
these types of flow in a manner that is anchored to actual data. In addition to comparisons with the shadowgraph data, we have performed detailed comparisons with the jet penetration data provided from the experiments. In each case, LES results are in good agreement with the experiments.

Having established quantitative agreement with the experiments, we performed detailed analysis of transient processes at the start of injection. The goal is to identify loss mechanisms that degrade the performance of the injector, to investigate the transient evolution of the mass flow rate through respective injector orifices, and to quantify the effect of injection pressure drop on the overall formation and quality of mixture during the injection process (see figure 3). Ongoing studies will include detailed analysis of the turbulent small-scale flow structure and the related scalar mixing processes, with emphasis placed on maximizing engine efficiency and minimizing emissions.

Calculations of the entire set of injectors are in progress. In addition to direct use of the model in a companion set of in-cylinder calculations, results from these studies will be used to systematically progress toward liquid hydrocarbon fuels. We will focus on (1) what is required to rigorously reproduce the essential broadband turbulent dynamics in the simulations using high-fidelity subgrid-scale models, (2) the accuracy that can be achieved through direct comparisons with key experimental data (see www.ca.sandia.gov/ecn), and (3) how the information provided by the high-fidelity models can be used for development of more affordable engineering models.

Acknowledgments
This work was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences. Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000. The work at Oak Ridge National Laboratory (ORNL) was supported by and used resources of the National Center for Computational Sciences (NCCS) at ORNL, supported by the DOE Office of Science under contract DE-AC05-00OR22725.

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