SAND2009-3721C

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

J. C. Oefelein[†], J. H. Chen[†] and R. Sankaran[‡]

[†]Reacting Flow Research Department, Sandia National Laboratories, Livermore, CA 94550

[‡]National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

E-mail: oefelei@sandia.gov

Abstract. There is an urgent and growing demand for high-fidelity simulations that capture complex turbulence-chemistry interactions in propulsion and power systems, and in particular, that capture and discriminate the effects of fuel variability. This project addresses this demand using the Large Eddy Simulation (LES) technique (led by Oefelein) and the Direct Numerical Simulation (DNS) technique (led by Chen). In particular, we are conducting research under the INCITE program that is tightly coupled with funded projects established under the DOE Basic Energy Sciences and Energy Efficiency and Renewable Energy programs that will provide the foundational science required to develop a predictive modeling capability for design of advanced engines for transportation. Application of LES provides the formal ability to treat the full range of multidimensional time and length scales that exist in turbulent reacting flows in a computationally feasible manner and thus provides a way to simulate reacting flow phenomena in complex internal-combustion engine geometries at device relevant conditions. Application of DNS provides a way to study fundamental issues related to small-scale combustion processes in canonical configurations to understand dynamics that occur over a range of reactive-diffusive scales. Here we describe the challenges and present representative examples of the types of simulations each respective tool has been used for as part of the INCITE program. We focus on recent experiences on the Oak Ridge National Laboratory (ORNL) National Center for Computational Sciences (NCCS) Cray-XT Platform (i.e., Jaguar).

1. Introduction

Turbulent combustion processes are prevalent in a wide variety of propulsion and power systems including internal-combustion (IC) engines, gas-turbines and liquid-rockets. As such, development and rigorous validation of science-based predictive models for turbulent combustion is recognized as an important priority in research and there are a variety of challenges. Turbulent flows involving heterogeneous chemically reacting mixtures (as is the case for all propulsion and power systems) have a variety of complicating factors including highly nonlinear chemical kinetics, small-scale velocity and scalar-mixing, turbulence-chemistry interactions, compressibility effects (volumetric changes induced by changes in pressure), and variable inertia effects (volumetric changes induced by variable composition or heat addition). Coupling between processes occurs over a wide range of time and length scales, many being smaller than can be resolved in a numerically feasible manner. Further complications arise when multiple phases are present due to the introduction of dynamically evolving interface boundaries and the complex exchange processes that occur as a consequence.

At the device level, high-performance, dynamic stability, low pollutant emissions, and low soot formation must be achieved simultaneously in highly confined geometries that generate extremely complex flow and acoustic patterns. Flow and combustion processes are highly turbulent (i.e., integral-scale Reynolds numbers of $\mathcal{O}(10^5)$ or greater), and the turbulence dynamics are inherently dominated

by geometry or various operating transients. In many cases operating pressures approach or exceed the thermodynamic critical pressure of the fuel or oxidizer. Operation at elevated pressures significantly increases the system Reynolds number(s) and inherently broadens the range of spatial and temporal turbulence scales over which interactions occur. The limitations and challenges associated simulating these phenomena requires that a hierarchy of approaches be taken to fully understand key processes and work toward predictive models. From this perspective, a hallmark of our combustion program is the interaction between theory, experiments, modeling, and simulations. Each approach complements the others. Here we highight two key research tools used toward this goal. The first is the solver developed by Oefelein *et al.* called RAPTOR [1–9]. The second is the solver developed by Chen *et al.* called S3D [10–15]. RAPTOR is a massively parallel flow solver designed specifically for application of the Large Eddy Simulation (LES) technique to turbulent, chemically reacting, multiphase flows. S3D is a massively parallel flow solver designed specifically for application of the Direct Numerical Simulation (DNS) technique. The combination of these techniques has enabled fundamental investigations of the fully coupled dynamic behavior of reacting flows with detailed chemistry. Following are representative results acquired from each as part of our DOE INCITE allocation.

2. Large Eddy Simulation

RAPTOR is a massively parallel flow solver designed specifically for application of LES to turbulent, chemically reacting, multiphase flows. It solves the fully coupled conservation equations of mass, momentum, total-energy, and species for a chemically reacting flow system (gas or liquid) in complex geometries. It accounts for detailed chemistry, thermodynamics, and transport processes at the molecular level and uses detailed chemical mechanisms. The code is sophisticated in its ability to handle complex geometries and a generalized subgrid-scale model framework. It is capable of treating spray combustion processes and multiphase flows using a Lagrangian-Eulerian formulation. The numerical formulation treats the compressible form of the conservation equations, but can be evaluated in the incompressible limit. The theoretical framework handles both multi-component and mixture-averaged systems. The baseline formulation employs a general treatment of the equation of state, thermodynamics, and transport properties that accommodates real gas or liquids with detailed chemistry (i.e., not constrained to ideal gas applications). Details are given by Oefelein [9].

As one example, we consider direct-injection (DI) processes for IC-engine applications. Direct injection has proven to be a promising option in Diesel and low temperature combustion 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 (which are an attractive alternative to fuel cells), DI provides the appropriate energy density required for high efficiency and low NO_x emissions. 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 engine operating conditions. In this work, we have developed a model for high-fidelity calculations of DI processes using LES and an advanced property evaluation scheme. The combination of High Performance Computing (HPC) and LES has significant potential to provide new insights into the dynamics of IC-engine flow processes, which is imperative for the development of next generation engines. The objective of this task is to fully integrate the combined merits of HPC and LES in a manner that provides some of the highest-fidelity, most detailed calculations ever performed to investigate turbulent reacting flow processes in IC-engines.

Recent calculations performed on the ORNL Cray-XT Platform (Jaguar) have been focused on detailed simulations of direct-injection (DI) processes in IC-engines, with emphasis on high-pressure processes relevant to low-temperature combustion applications. Fundamental high-fidelity representations of DI processes in IC-engines are an essential component toward the development of a validated predictive modeling capability. However, detailed models are still lacking and few provide a rigorous description of transient processes that occur between the jets and the in-cylinder flow environment as fuel is injected into an engine. As part of our 2008-2009 INCITE award, we have

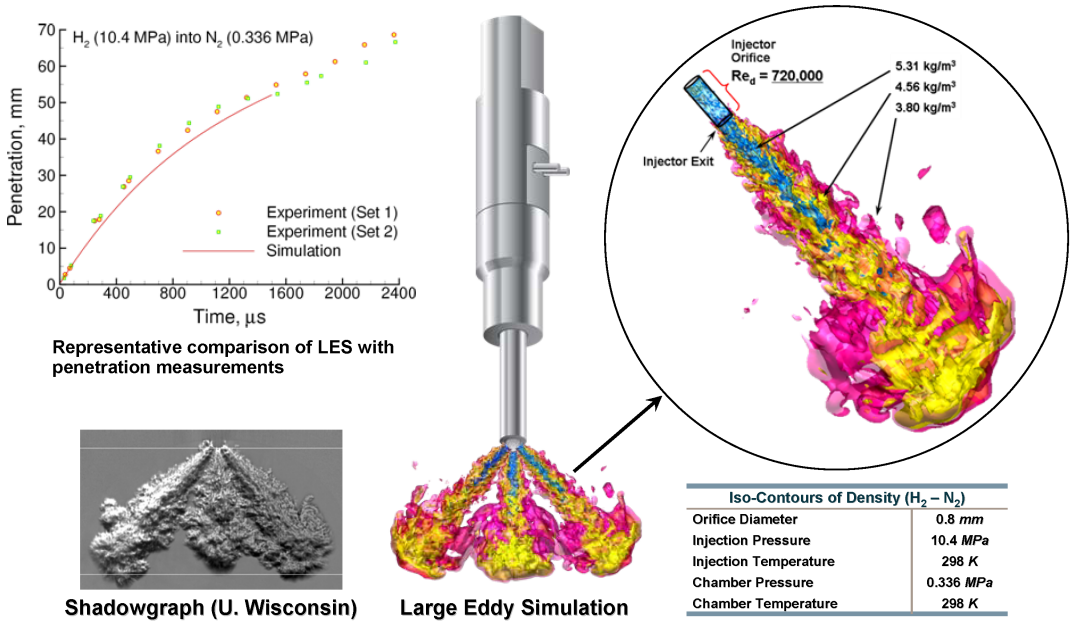

Figure 1: LES of high-pressure injection processes under actual operating conditions. To the left are penetration measurements and a corresponding shadow graph image acquired experimentally. In the center is a representative LES calculation at identical conditions showing the complete computational domain. To the right is an enlargement of one of the jets showing the turbulent structure at an instant in time.

performed one of the highest fidelity simulations of DI processes ever as a precursor to a full engine simulation (which will also be performed as part of our INCITE grant). Figure 1 shows a representative result, which has been validated using experimental data from the University of Wisconsin (see T.G. Drozda and J.C. Oefelein (2008). Large eddy simulation of direct injection processes for hydrogen and LTC engine applications. SAE World Congress, Paper 2008-01-0939). To the left of the figure are penetration measurements made experimentally along with our predicted results (which show the rate at which the fuel is injected into the engine) and a corresponding shadowgraph image (which shows the transient structure of the turbulent jets). In the center is the corresponding LES calculation showing the complete computational domain, which is an actual 3-orifice injector used in the optical engines at the Combustion Research Facility. To the right is an enlargement of one of the jets showing the turbulent structure in both the injector orifice and the ambient environment at an instant in time. The calculation was performed by gridding the entire injector, including the internal flow passages and needle valve actuator that controls the flow of fuel. A key issue in modeling flows at actual conditions is the fact that they exhibit extremely high Reynolds numbers. For the calculations performed here, the jet Reynolds number is 720,000. These studies are precursor calculations to a more detailed set of simulations that are currently being conducted in a full internal combustion engine. The objective is to identically match the operating conditions and geometry and in so doing establish a direct collaboration with our experimental efforts at the Combustion Research Facility.

3. Direct Numerical Simulation

Petascale simulations provide a way to study fundamental issues related to small-scale combustion processes in well-defined laboratory configurations, in environments where measurements are difficult or impossible to obtain. As one example, we have performed DNS of a lifted ethylene-air jet flame with emphasis placed on stabilization in a heated coflow. The objective was to understand how a lifted autoignitive flame is stabilized in a canonical configuration with relevance to diesel jet flame stabilization.

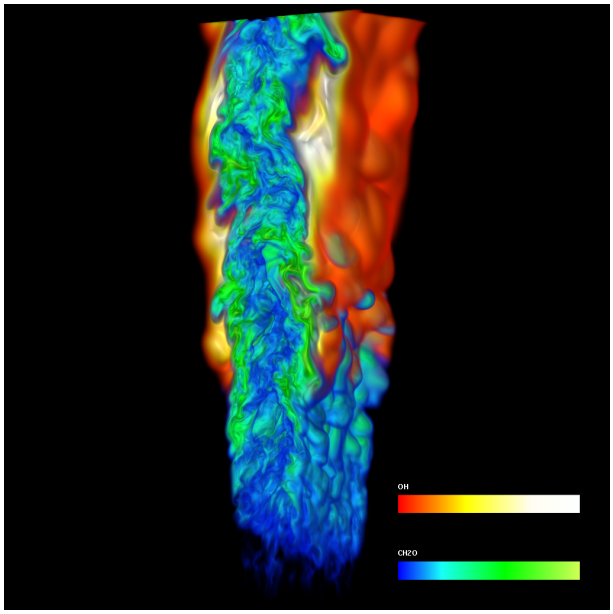

Figure 2: DNS of a lifted ethylene-air jet flame at Reynolds Number 10,000. The hydroxyl radical (red/white) denotes the lifted flame whereas formaldehyde (blue/green) denotes ignition intermediates upstream of the lifted flame.

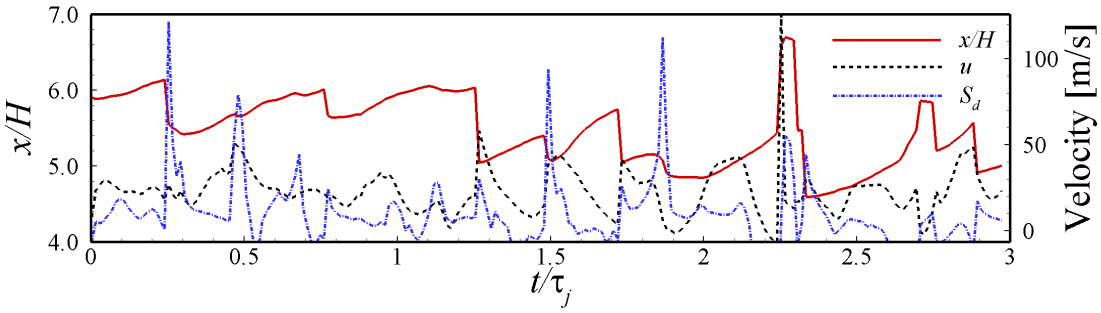

Figure 3: Time history of the axial fluctuation in the flame stabilization height, x/H, where H is the jet height, the local axial gas velocity (u) and the displacement speed of the stabilization point (S_d).

DNS of the near field of a three-dimensional spatially-developing turbulent lifted jet flame in a 1550K heated air coflow was performed with a reduced ethylene-air mechanism (22 species; 18 global steps; 167 reactions) [16] to determine the stabilization mechanism. The DNS was performed at a jet Reynolds number of 10,000 with 1.28-billion grid points. The results reveal that auto-ignition in a fuel-lean mixture immediately upstream of the flame base is the main source of stabilization of the lifted jet flame. This is verified by the presence of a key ignition precursor, HO_2, along with low levels of CH_3, OH and CH_2O upstream of where the flame is established as shown in the instantaneous image in Fig. 2. The dynamics of the fluctuations in the lifted flame stabilization point are studied by temporal tracking of the most upstream point where the hydroxyl radical is observed at a threshold of 5 percent of its peak value in the domain. The fluctuations of the flame lift-off height and the local gas and flame displacement speed are shown in Fig. 3. Large displacement speeds (i.e greater than 100 m/s) in excess of the laminar flame speed are indicative of spontaneous ignition. As well, the fast front propagation speed is accompanied by a rapid motion of the lift-off height upstream, similar to observations made in a lifted hydrogen/air jet flame [17]. Fundamental understanding of this issue, provided by detailed scalar and velocity statistics from the DNS, and many others is needed to develop robust and reliable combustion models for the

combustion regimes observed under low-temperature combustion engine environments.

As a second example, we have performed DNS of ignition processes in a lean n-heptane/air mixture under HCCI conditions with temperature inhomogeneities. Homogeneous charge compression-ignition (HCCI) engines have been considered as an alternative for diesel and spark-ignition (SI) engines because HCCI engines can provide high efficiencies and very low NO_x and particulate emissions. However, under high-load HCCI operation, a high-rate of pressure rise during combustion can result in damaging engine knock. Thermal stratification induced by temperature inhomogeneities in engines has been proposed as a control measure for too rapid a pressure rise rate by spreading out the heat release through mixture preparation. To understand the effect of the thermal stratification on HCCI combustion characteristics, we performed two-dimensional DNS of lean n-heptane/air mixture ignition at constant volume with temperature inhomogeneities. As in hydrogen/air mixture ignition under HCCI conditions [18], large temperature fluctuations spread out the mean heat release rate and reduces its peak during both ignition stages. However, the overall heat release rate during the second-stage ignition is retarded as the temperature fluctuation increases. This fact will become important as we move forward and consider a variety of alternative fuels with wide variations in ignition characteristics. In addition, the effect of different temperature fluctuation length scales, larger temperature fluctuation RMS, equivalence ratio fluctuations, different turbulence time scales, and addition of EGR will be investigated. Several three-dimensional DNS studies will be performed to provide statistics for mixing and ignition model development and validation.

4. Acknowledgments

This work was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences and the Office of Vehicle Technologies. 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. Computer time was granted under the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.

References

[1] Oefelein J C and Sankaran R 2009 *Proceedings of the 21st International Conference on Parallel Computational Fluid Dynamics* Moffett Field, California
[2] Frank J H, Kaiser S A and Oefelein J C 2009 *Proceedings of the 6th Joint Meeting of the US Sections of the Combustion Institute, Paper 32D1* Ann Arbor, Michigan
[3] Sankaran V, Drozda T G and Oefelein J C 2009 *Proceedings of the Combustion Institute* **32** 1571–1578
[4] Oefelein J C 2008 *IFP Workshop on Large Eddy Simulation for Internal Combustion Flows* Ruell-Malmaison, France
[5] Drozda T G and Oefelein J C 2008 *SAE World Congress, Paper 2008-01-0939* Detroit, Michigan
[6] Drozda T G, Wang G H, Sankaran V, Mayo J R, Oefelein J C and Barlow R S 2008 *Combustion and Flame* **155** 54–69
[7] Williams T C, Schefer R W, Oefelein J C and Shaddix C R 2007 *Review of Scientific Instruments* **78** 035114–1–9
[8] Oefelein J C, Sankaran V and Drozda T G 2007 *Proceedings of the Combustion Institute* **31** 2291–2299
[9] Oefelein J C 2006 *Progress in Aerospace Sciences* **42** 2–37
[10] Hawkes E R, Sankaran R, Chen J H, Kaiser S and Frank J H 2009 *Proceedings of the Combustion Institute* **32** 1455–1463
[11] Richardson E S, Yoo C S and Chen J H 2009 *Proceedings of the Combustion Institute* **32** 1695–1703
[12] Lignell D, Chen J H and Smith P J 2008 *Combustion and Flame* **155** 316–333
[13] Sankaran R, Hawkes E R, Chen J H, Lu T and Law C K 2007 *Proceedings of the Combustion Institute* **31** 1291–1298
[14] Cook D J, Pitsch H, Chen J H and Hawkes E R 2007 *Proceedings of the Combustion Institute* **31** 2903–2911
[15] Sutherland J C, Smith P J and Chen J H 2007 *Combustion Theory and Modelling* **11** 287–303
[16] Lignell D O, Chen J H, Smith P J, Lu T F and Law C K 2007 *Combustion and Flame* **151** 2–28
[17] Yoo C S, Chen J H and Sankaran R 2009 *Journal of Fluid Mechanics* In Press
[18] Hawkes E R, Sankaran R, Pebay P P and Chen J H 2006 *Combustion and Flame* **145** 145–159