DNS of Turbulent Combustion Towards Fuel-Flexible Gas Turbines and IC Engines

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First principles Direct Numerical Simulation of turbulent combustion shed light on underlying turbulence-chemistry interactions relevant to the design of next-generation fuel-flexible stationary gas turbines and fuel-efficient, clean internal combustion engines using biofuels. A suite of DNS benchmarks was performed that is enabling the development of predictive models for lifted diesel flame stabilization, discerning flame and ignition propagation in dual-fuel reactivity controlled compression ignition combustion, and ensuring intrinsic flashback safety in fuel injection systems for fuel-flexible gas turbines.

Projections of global energy utilization ensure that combustion will continue to be the predominant mode of energy conversion for transportation, power generation, and industrial thermal processes for the next half-century. Considerations of energy and environmental security and sustainability, as well as economic competitiveness, demand accelerated development of advanced combustion technologies that combine high efficiency, low emissions, and the ability to reliably operate on an increasingly diverse range of fuels, including bio-derived and synthesis fuels, as well as an evolving feed of fossil fuels. Development of these technologies are significantly hampered by the lack of robust, predictive computational design tools for advanced combustion systems, particularly in new mixed-mode combustion regimes where stringent efficiency and emissions legislation are driving future technologies.

In the past year we have performed a suite of canonical laboratory-scale DNS targets with our INCITE award at OLCF that were carefully designed to shed light on fundamental ‘turbulence-chemistry’ interactions relevant to the design of next-generation fuel-flexible stationary gas turbines and internal combustion engines. These are described below:

1) Turbulent lifted autoignitive di-methyl ether jet flame at moderate pressure

Injection of a turbulent fuel stream issuing into a hot, vitiated, oxidizing environment, followed by autoignition and lifted flame stabilization underpins a significant number of advanced engine systems, most notably low-temperature diesel engines. Recent DNS studies have shown the influence of high-temperature auto-ignition on lifted flame stabilization in stationary H_2/air and C_2H_4/air jet flames at ambient pressure, while the role of low-temperature pre-ignition on lifted jet flame stabilization at high pressure is still not understood. Furthermore, DNS of a laminar lifted DME jet flame shows the presence of distinct pentabrachial structures not seen before. Also, the effect of low-temperature, cool flame reaction progress in a mixing field established by turbulent jet on lifted flame stabilization is not understood. Hence, we have performed DNS of a lifted turbulent DME jet flame to investigate the dynamic coupling between turbulent mixing fluctuations and autoignition ; the influence of low-temperature, pre-ignition chemistry on lifted flame stabilization; and the resulting detailed turbulent flame structure at moderate pressures.

2) Effect of fuel composition and differential diffusion on flame stabilization in reacting syngas jets in turbulent cross-flow

Several technical challenges remain in the development of a combustion system capable of efficient, clean and safe combustion of Integrated Gasification Combined Cycle (IGCC) syngas: in particular, the often varying composition of the fuel, that can contain large fractions of hydrogen, must be taken into account at the combustor design stage, especially if the system must comply with the emissions regulations for threshold levels of CO and NOx and also ensure intrinsic flashback safety. There are a number of outstanding issues involving complex interactions between the flow field, mixing and reaction kinetics associated with fundamental fuel injection combustion processes that are not well understood and measurements are limited. Hence, we have performed three-dimensional DNS of a transverse syngas fuel jet in a turbulent boundary layer cross-flow of air to understand the influence of different syngas compositions (ratio of CO to H2) on the near field flame stabilization.

3) High productivity computing: turbulent combustion simulation of reactivity controlled compression Ignition with a primary reference fuel using Legion

Direct numerical simulation of turbulent combustion is an important tool for understanding the performance of fuels used in internal combustion engines. We performed the first large-scale 3D direct numerical simulation of dual fuel reactivity controlled compression ignition with a realistic primary reference fuel (PRF) blend of iso-octane and n-heptane, involving 116 chemical species and 861 reactions. The DNS results showed the presence of mixed modes of combustion including both spontaneous autoignition and premixed flame propagation. The DNS data provides a unique benchmark for the development and validation of mixed-regime models.

Our results were achieved using Legion, a novel task-based programming system. Legion automates details of scheduling tasks and data movement, and separates the specification of tasks and data from the mapping onto a machine. We refactored our

DNS code, S3D, in Legion and demonstrated these properties of Legion have profound implications for programmer productivity, shortening porting and tuning activities previously requiring weeks down to hours. Our project required changes in functionality, ports to multiple supercomputers including both Titan and Piz Daint, 2-D vs. 3-D simulations, and low vs. high resolution runs. Each variation alters both work and communication, sometimes radically, but remapping using Legion required minimal human effort. The result is a robust, easily modified PRF implementation that improves time to solution by nearly 9X and obtains over 80% of the achievable performance on both target systems.