Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry: Spray Simulations

Final Report: March 2009
DOE Award: DE-FG02-01ER15234

Engine Research Center
University of Wisconsin – Madison
Professor Christopher J. Rutland

Project Summary

The Terascale High-Fidelity Simulations of Turbulent Combustion (TSTC) project is a multi-university collaborative effort to develop a high-fidelity turbulent reacting flow simulation capability utilizing terascale, massively parallel computer technology. The main paradigm of the approach is direct numerical simulation (DNS) featuring the highest temporal and spatial accuracy, allowing quantitative observations of the fine-scale physics found in turbulent reacting flows as well as providing a useful tool for development of sub-models needed in device-level simulations. Under this component of the TSTC program the simulation code named S3D, developed and shared with coworkers at Sandia National Laboratories, has been enhanced with new numerical algorithms and physical models to provide predictive capabilities for turbulent liquid fuel spray dynamics. Major accomplishments include improved fundamental understanding of mixing and auto-ignition in multi-phase turbulent reactant mixtures and turbulent fuel injection spray jets.

Program Scope

The primary goal of the SciDAC TSTC was to extend the S3D code with enhanced physical and algorithmic modules, and undertake several large-scale simulations to investigate important scientific issues. The task for the Spray Simulation component of the TSTC project was to develop a spray module for the S3D DNS code to elevate its capability to deal with liquid fuel droplets. The ultimate target is to understand the mechanism of spray combustion and its dependency on droplet evaporation, turbulence mixing and ignition, so as to provide insight into the factors dominating the combustion processes in diesel and other direct injection engines. Fuel droplets are tracked by the Lagrangian method. Full two-way coupling interaction between the gaseous phase and fuel droplets is expressed by mass, momentum and energy transfers. The specific objectives of this component of the project include:

- To enhance the computational architecture and numerical algorithms in order to allow more robust, accurate, and efficient simulations of multi-dimensional, multi-phase turbulent combustion in the presence of strong turbulence and chemical stiffness. The efforts include new algorithms for Lagrangian droplet transport and phase change, chemical reaction source terms and improved code architecture for various hardware platforms.

- To expand and upgrade the physical submodels to describe the underlying mechanisms in greater detail. Modules to simulate liquid spray fuel injection were developed and integrated into the S3D code

Partnership

The TSTC project was originally launched in 2001 as part of the DOE Scientific Discovery through Advanced Computing (SciDAC) program in order to address the complexities and challenges associated with performing first-principles numerical simulations of turbulent combustion on massively parallel computing architectures. Recognizing these challenges, a consortium of research institutions (University of Maryland, University of Michigan, University of Wisconsin, Sandia National Laboratories, Pittsburgh Supercomputing Center) was established in TSTC Phase I (2001-04) to achieve a critical mass of interdisciplinary skills and to develop a scalable, massively parallel DNS solver for turbulent combustion. The partnership was renewed in TSTC Phase II (2004-07), but without Pittsburgh Supercomputing Center. During TSTC Phases I and II, the DNS solver S3D has been re-designed for effective use on terascale high-performance computing platforms, as well as enhanced with new numerical and physical modeling capabilities.

As part of the 2005 Joule Software Effectiveness study, S3D was ported to the Cray X1 and XT3 platforms at the NCCS/ORNL. Furthermore, several key modules of S3D were optimized and rewritten to improve the performance of the code on different platforms. As a result, the performance improved by 45% on the scalar architectures. The new modules were also suitable for vectorization, which enabled a terascale combustion science simulation on the Cray X1E.

Accomplishments

To understand the mechanism of spray combustion and its dependency on droplet evaporation, turbulence mixing and ignition, a spray module was developed. The module includes full coupling between gas and liquid phases for evaporating sprays. A Lagrangian method is employed to track the individual droplets, and is embedded into the Eulerian framework for the gas-phase flow in S3D. The spray model adopts the classical PICell (Particle-In-Cell) method (a method that is widely used in the field of spray/particle fluid dynamics); it also uses a fourth-order interpolation scheme to identify the local gas properties at the droplet location and a general method to distribute the source terms according to an arbitrarily defined basis function, such that the distribution of drop source terms is smooth and independent of the grid size.

Fundamental simulations using DNS type procedures were used to investigate the ignition, combustion characteristics and the lift-off trends of a spatially evolving turbulent liquid fuel jet. In particular, a spatially evolving n-Heptane spray injected in a two-dimensional rectangular domain with an engine like environment was investigated. The computational results were compared to experimental observations from an optical engine as reported in the literature. It was found that an initial fuel rich combustion downstream of the spray tip is followed by diffusion combustion. Investigations were also made to understand the effects of injection

velocity, ambient temperature and the droplet radius on the lift-off length. For each of these parameters three different values in a given range were chosen. For both injection velocity and droplet radius, an increase resulted in a near linear increase in the lift-off length. An increase in the ambient temperature resulted in a decrease in the lift-off length.

Isotropic Simulations Before simulating liquid sprays, a study of n-heptane liquid drops in isotropic turbulence was performed. The n-heptane chemical reactions were simulated using a validated and moderately detailed kinetics mechanism using 44 species and 112 reactions. A two-dimensional square domain of 1.2 cm by 1.2 cm and a grid with 192 by 192 points were used in the simulations (Δx = 62.5 μm). Five cases were simulated in total. The initial gas pressure for all cases is six atmospheres. Three different initial gas temperatures were used: 1100 K, 1200 K and 1300 K. Three global equivalence ratios of 0.5, 1.0, and 1.5 were simulated.

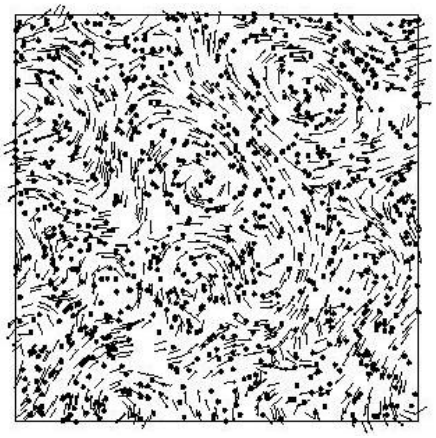

Fig. 1 Initial gas velocity vectors and distribution of droplet locations (only 5% of the velocity vectors are shown for clarity).

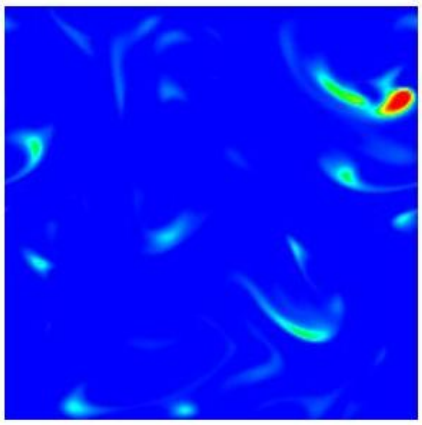

Fig. 2 Temperature contour at t=0.89 ms for the T= 1300 K case (Blue=1500 K; Red=2000 K).

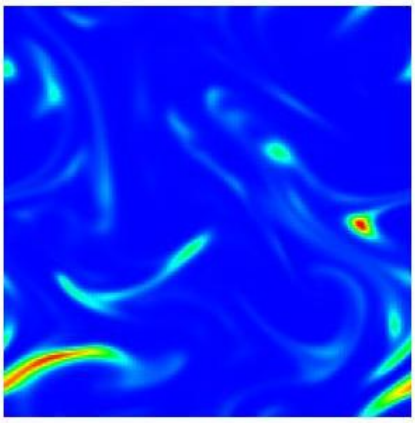

Fig. 3 Contour of the equivalence ratio at t = 0.89 ms (Blue = 0.0; Red = 0.08) for the T= 1300 K case.

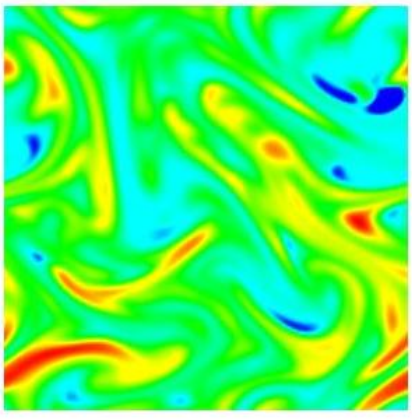

Fig. 4 Contour of C_2H_4 mass fraction at t=0.89 ms for the T= 1300 K case (Blue=0.0; Red=0.023).

An example of the initial gas velocity vectors and distribution of droplet locations are shown in Fig. 1. The general character of the turbulent simulations is shown in contour plots of

temperature, equivalence ratio, and C_2H_4 mass fractions in Figs. 2-4. This is for the case with initial T = 1300 K and global equivalence ratio of 0.5 at a time of 0.89 ms. At this time all of the drops have evaporated, several ignition kernels are developing, and global thermal runaway is imminent. The equivalence ratio (Fig. 3) is calculated using the base fuel concentration (n-heptane) and shows that most of the fuel has reacted to form ignition intermediate species. Figure 4 shows a major intermediate, C_2H_4, is prevalent through the domain except where it has been depleted in the ignition kernels. This figure also shows the strong non-uniformity of C_2H_4 caused by the distributed droplet sources and the turbulent mixing. Distributions for other cases are similar, but with higher uniformity for longer ignition delay times. The general process in this, and all other cases, is: (i) the fuel droplets evaporate quickly, (ii) there is a period of mixing and low temperature reactions, (iii) ignition occurs at a few sites, and (iv) then combustion over the complete domain occurs very rapidly.

Fuel Spray Simulations In diesel engines, the reaction zone of a diesel spray stabilizes at a location downstream of the injector orifice at the end of the auto-ignition phase. This distance is referred to as the lift-off length and is critical in determining the extent to which the fuel and air premix upstream of this distance. This in turn influences the combustion phasing and efficiency, and the formation of soot.

Simulations of a turbulent fuel spray injection under diesel like conditions were made. Figure 5 shows contours of temperature at the time of ignition. Ignition kernels form on the periphery of the liquid jet consistent with experimental results. Ignition occurs at locations of low scalar dissipation rate, lean mixture fraction, and low vorticity magnitude.

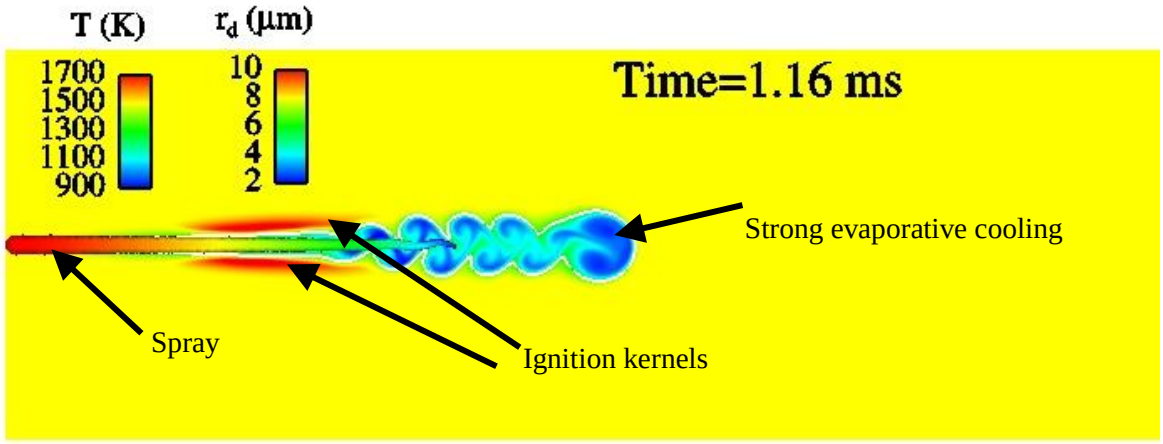

Figure 5: Temperature contours at the time of ignition for the spatially evolving spray jet. Contour colors indicate temperature and droplet sizes as they are injected at the left boundary. (T_{amb}: 1500 K, P_{amb}: 1 atm, nozzle diameter 0.2 mm, fuel injection: 100 m/s, 20 μm drop diameter)

After ignition, the flame kernels spread both upstream and downstream. This 'spreading' does not appear to be conventional flame propagation. Instead it may be similar to the spontaneous flame propagation due to pre-existing reaction and temperature gradients. The result is shown

in Fig. 6 where nearly stationary lifted flames are established near the injection location, and flamelets propagate downstream following the stoichiometric surface.

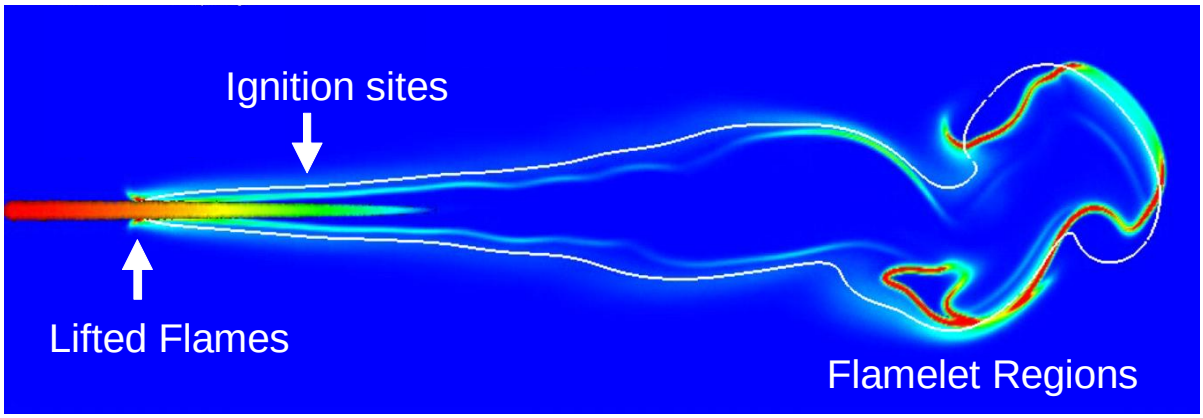

Figure 6: Heat release contours of combustion in the evolving fuel spray jet. The liquid jet is shown at the left by droplets colored by their temperature. The white line denotes the stoichiometric line. At this time (2.60 ms), ignition kernels have evolved into lifted flames near the injector and propagating flames in the downstream, spray plume region.

A series of DNS simulations were made for understanding the flame lift-off length characteristics. Simulations were made for three different injection velocities, ambient temperatures and droplet radii and their influence on the lift-off length was studied. The results were compared to the experimental investigation from the literature. It was found that:

1. The lift-off length varies linearly with respect to the injection velocity. This variation is similar to the one observed by Siebers et. al [1] and is attributed to the turbulent mixing effects which increase with increase in velocity, forcing the flame stabilization downstream (c.f. Figure 7).

2. In the regime of ambient temperatures (1400K-1500K) that was tested in this study, the lift-off length is proportional to temperature to the -3.74 power (c.f. Figure 8). This trend was also observed in the experimental investigations of Siebers et. al[1]. This occurs because with an increase in ambient temperature the evaporation rate of the droplets increases. As a result of this, larger quantities of evaporated fuel are available which allow the stable combustion point to occur further upstream for higher ambient temperatures. Also, with an increase in temperature the combination of increased thermal diffusivity and flame speed resulted in a faster local flame reaction rate which causes the flame to stabilize closer to the injector.

3. An increase in droplet radius resulted in a linear increase in the lift-off length (c.f. Figure 10). Experimental investigations on the orifice diameters (which impact the droplet sizes) have

[1] D. L. Siebers and B. Higgins, "Flame Lift-Off on Direct-Injection Diesel Sprays Under Quiescent Conditions," SAE Technical Paper 2001-01-0530 (2001). and D. L. Siebers, B.S. Higgins and L. M. Pickett, "Flame Lift-Off on Direct-Injection Diesel Fuel Jets: Oxygen Concentration Effects," SAE Technical Paper 2002-01-0890 (2002).

shown the lift-off length to be proportional to the 0.34 power of the orifice diameter over a broad range of the diameters. Since, in this study a relatively small range of droplet radius (15-25µm) was used, a local linearization that has been observed is a good approximation to the same trend. A combination of higher momentum and lower evaporation rate results in an increased spray penetration, forcing the flame stabilization further downstream when the droplet radius is increased.

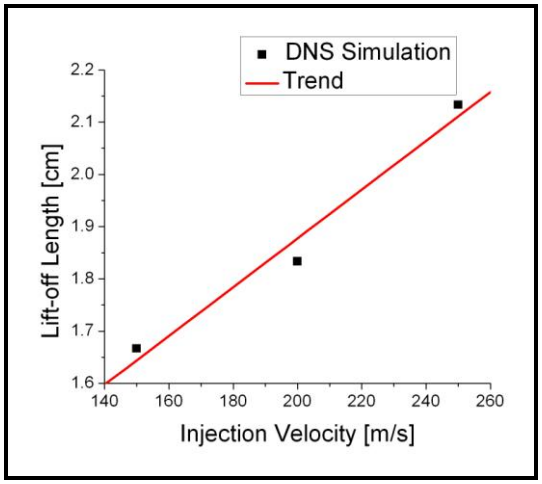

Figure 7: Lift-off length for three injection velocities (150m/s, 200m/s and 250m/s) of an n-heptane jet. The square symbols are the three DNS measurements. The line represents the linear trend with a slope of 0.05cm/mps

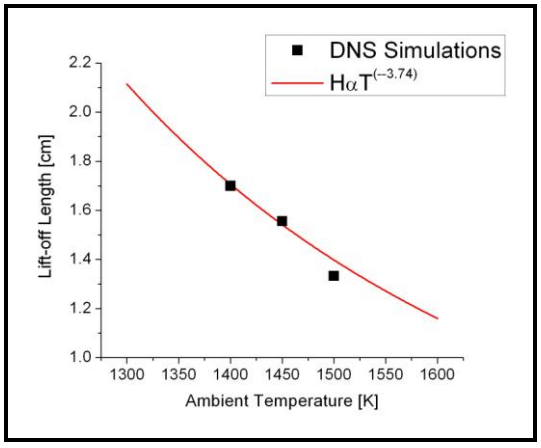

Figure 8: Lift-off length for three ambient temperatures (1400K, 1450K and 1500K) for a n-heptane jet. The square symbols are the three DNS measurements. The line represents the decaying trend of $H \propto T^{-3.74}$.

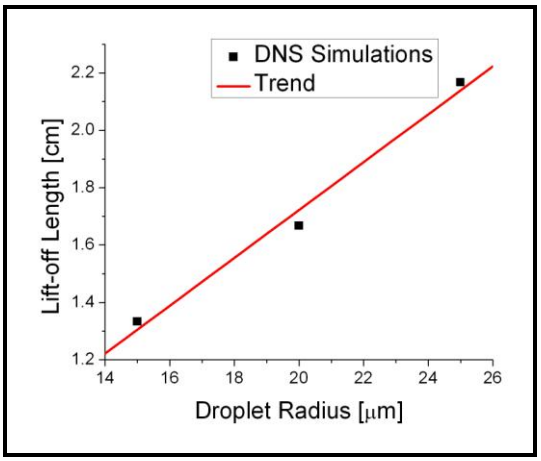

Figure 9: Lift-off length for three droplet radii (15μm, 20μm and 25μm) for a n-heptane jet. The square symbols are the three DNS measurements. The line represents the linear trend with a slope of 0.0834cm/μm.

Summary

An advance spray module was developed and added to the S3D DNS code for the study of ignition and combustion in turbulent reacting multi-phase flows, including fuel injection sprays. The module was used to ignition in isotropic turbulent flows and diesel-like fuel injection flows. This has provided improved understanding of technologically important direct injection fuel applications. This work is currently being used to help develop large eddy simulation (LES) spray models for use in studying advanced engine combustion technologies.

Project Publications

1. Wang, Y. and C. J. Rutland, 2003, "On the Combustion of Normal Heptane Fuel Droplets in Isotropic Turbulence with DNS", *Proceedings of the Third Joint Meeting of the U.S. Sections of The Combustion Institute*, March 2003, Chicago, IL.

2. Wang, Y. and C. J. Rutland, 2005, "Effects of temperature and equivalence ratio on the ignition of n-heptane fuel droplets in turbulent flow." *Proceedings of the 30th International Symposium on Combustion*, Vol. 30:893-900.

3. Wang, Y., and C.J. Rutland, 2006, "Direct numerical simulation of turbulent flow with evaporating droplets at high temperature," *Heat and Mass Transfer*, Vol. 42, No. 12, pp. 1103-1110.

4. Wang, Y. and C. J. Rutland, 2007, "Direct numerical simulation of ignition in turbulent n-heptane liquid fuel spray jets," *Combustion and Flame* 149, pp 353-365.

5. Srinivasan, S. and C.J. Rutland, 2007, "Combustion and Lift-off Characteristics of n-Heptane Sprays Using Direct Numerical Simulations", *SAE Technical paper 2007-01-4136*

6. Srinivasan, S. and C.J. Rutland, 2008, "Effects of EGR Components Along with Temperature and Equivalence Ratio on the Combustion of n-Heptane Fuel", Seshasai Srinivasan and Christopher Rutland, *SAE Technical paper 2008-01-0951*.

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7. Wang, Y.and C. J. Rutland, 2005, "DNS study of the ignition of n-heptane fuel spray under high pressure and lean conditions," *J. of Physics: Conference Series (SciDAC)*, Vol. 16, pp. 124-128.

8. Rutland, C.J. and Y. Wang, 2006, "Turbulent liquid spray mixing and combustion – fundamental simulations," *J. of Physics: Conference Series (SciDAC)*, Vol. 40, pp. 28-37.

Conferences

9. Wang, Y. and Rutland, C. J. (2003), "On the combustion of normal heptane fuel droplets in isotropic turbulence with DNS," *3rd Joint Meeting of the US Sections of the Combustion Institute*, Chicago, IL.

10. Wang, Y. and Rutland, C. J. (2003), "Direct numerical simulation of turbulent droplets flow with evaporation," *The 41st AIAA Aerospace Sciences Meeting and Exhibit*, AIAA Paper 2003-1281, 6-9 January 2003, Reno, Nevada, USA.

11. Wang, Y. and Rutland, C. J. (2004), "Effects of droplet velocity and size on the ignition of n-heptane fuel spray in turbulent flow using DNS." *Tenth SIAM International Conference on Numerical Combustion*, May 9-12, Sedona, AZ.

12. Wang, Y. and Rutland, C. J. (2004), "Effects of temperature and equivalence ratio on the ignition of n-heptane fuel droplets in turbulent flow," *30th International Symposium on Combustion*, July 25-30, Chicago, IL.

13. Wang, Y. and Rutland, C. J. (2004), "DNS study of the ignition of n-heptane fuel spray under HCCI condition," *57th APS Annual Meeting of the Division of Fluid Dynamics*, Seattle, WA, November.

14. Wang, Y. and Rutland, C. J., 2005, "On the Ignition of Turbulent Liquid Fuel Spray Jets using Direct Numerical Simulation," *58th APS Annual Meeting of the Division of Fluid Dynamics*, Chicago, IL, November 20-22.

15. Seshasai Srinivasan, Rutland, C.J., and Wang, Y., (2006) "Fundamental Simulations of Mixing and Combustion of Turbulent Liquid Sprays," *IEA Combustion Agreement, 2007 Conference*, Detroit, MI, April 14, 2007.