교내 슈퍼컴퓨팅을 활용한 연구

High-Fidelity Direct Numerical Simulations of Reacting Flows

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As global warming and air pollution worsen and the fossil fuel shortage becomes eminent in the near future, the demand for renewable energy and clean and efficient combustion has grown significantly. Before jumping into the discussion of details of combustion study, it is of interest to note that combustion accounts for approximately 90 % of total energy usage worldwide and the transportation accounts for 3/4 of petroleum usage in US (see Fig. 1). Astonishingly, the renewable energy,including biofuels, solar photovoltaic, wind, solar heat and etc, covers only 1 % of total energy usage in the world, implying that a more intensive research of renewable energy should be done in the near future. Together with this, the development of clean and efficient combustionengines should be another target to meet the energy demand in theforeseeing future. Simply speaking, 1 % efficiency gain of combustion engines is comparable to 100 % increase of the renewable energy development.

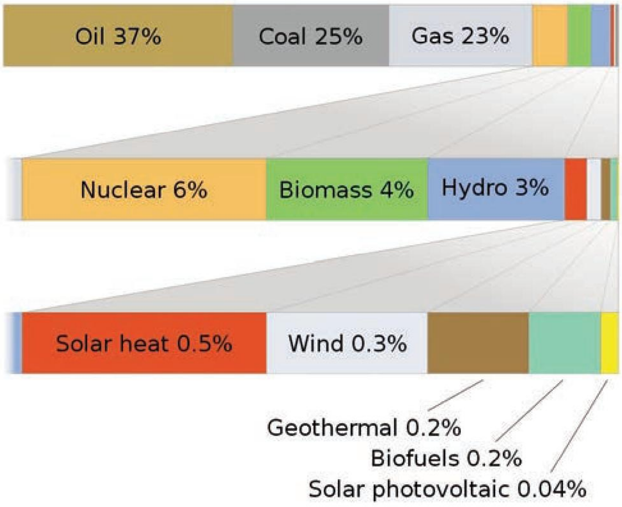

Figure 1. Total energy usage worldwide

To meet the demand, several new combustion technologies have been proposed thus far. Low-temperature combustion(LTC) has drawn a great attentionbecause it usually operates under fuel-lean conditions to avoid the generation of soot and NO_x as shown in Fig. 2. One of the examples of LTC is homogeneous charge compressionignition(HCCI) engines, whichhaveemerged as an alternative to conventional diesel and spark-ignition engines due to its high diesel-like fuel efficiency with low emission.

Figure 3 shows a schematic of HCCI engine concept which utilizes the advantages of the premixedness of spark-ignition(SI) engines and the high compression-ratio of compression ignition(CI) engines. HCCI engines are also characterized by low-temperature combustion and ultra-low emission(< 1900 K). As indicated in the BES report(Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels(2006), available from (http://science.energy.gov/~/media/bes/pdf/reports/files/ctf_rpt.pdf), HCCI combustion occurs primarily through volumetric autoignition, largely in the absence of flames under lean, dilute, high-pressure and low-temperature conditions. Therefore, HCCI combustion is primarily controlled by chemical kinetics of the fuel-air mixture.

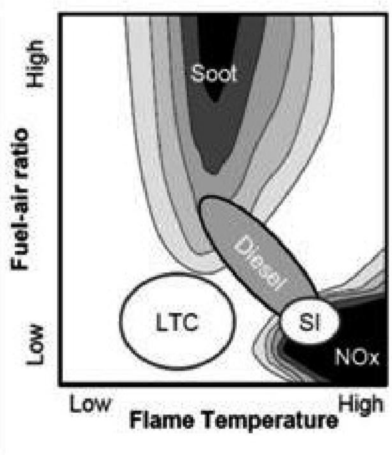

Figure 2. Operating regimes of traditional Spark-Ignited(SI) gasoline engines, Diesel engines, and novel low temperature combustion(LTC) devices which aim at creating conditions where the formation of soot and nitrogen oxides is avoided.

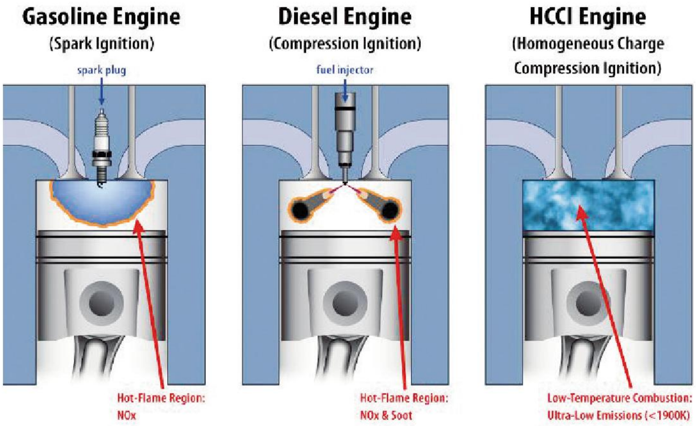

Figure 3. Schematic of homogeneous charge compression ignition (HCCI) engines

In addition, a new technology utilizing hydrogen jets issuing into a hot environment hasalso been proposed to meet the more stringent regulations of NO_x emission in gas turbines.Compared to current engines, combustion processes in these new technologies can be characterized by much higher pressure, lower temperature, and higher levels of dilution air. However, combustion processes in these environments have not been fully understood due to the limitations of experimentsand simulations.

Since the beginning of the new millennium, however, direct numerical simulations(DNS) of laboratory-scale turbulent jet flames can now be simulated with detailed kinetic mechanisms in three dimensions and provide a first-principles understanding of such turbulent flames and a database for turbulent combustion modeling. This is primarily attributed to the development of high-performance computing(HPC) clusters and novel numerical methods. DNS is one of the CFD(computational fluid dynamics) approaches in the continuum level, adopting a very fine grid such that it does not require any turbulence models but does need a huge amount of computational resources, especially for 3-D DNS.

In the combustion and propulsion laboratory, we have studied the stabilization mechanisms of laboratory-scale turbulent lifted jet flames in heated coflows and the ignition and combustion characteristics of high hydrocarbon fuel/air mixtures under HCCI conditions using DNS. Inaddition, weare also in vestigating the cellular instability of tubular and counterflow flames.

1. TurbulentLifted Jet Flames

Turbulent lifted jet flames in heated coflow have been widely investigated not only because of their practical importance in commercial applications such as diesel engines and gas turbine combustors, but because of fundamental importance for understanding auto-ignition and partial premixing in turbulent combustion modeling.

After state-of-the-art 3-DDNS of turbulent lifted hydrogen jet flame in heated coflow was performed, the trilogy of 3-D DNS of turbulent lifted jet flames in heated coflows have been performed and their stabilization mechanisms have been elucidated (see Fig. 4). The DNS were performed on Cray XT3-5 (Jaguar) in Oak Ridge National Laboratories using a compressible DNS code, S3D. From the studies, the stabilization mechanisms and flame structures are elucidated depending on the coflow temperature and velocity. These DNS cases are now being used for development and validation of turbulent combustion models

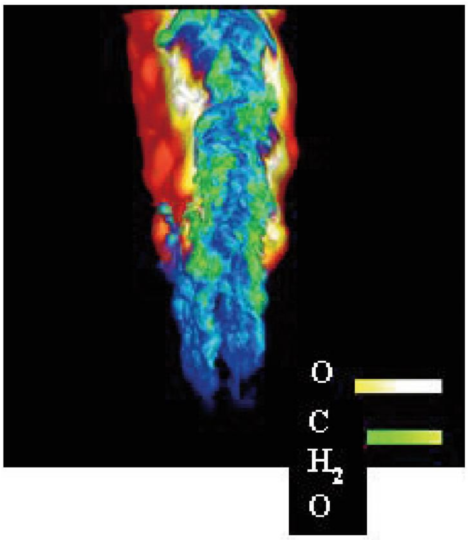

Figure 4. 3-D volume rendering of OH and CH_2O mass fractions of turbulent lifted ethylene jet flame in a high lyheated coflow

2. HCCI combustion

Up to now, one of the key issues in the development of HCCI engines is how to control the ignition timing and the excessive rate of pressure rise under wide range of load conditions. In particular, an excessive rate of pressure rise under high-load condition can result in engine knock, reducing the engine integrity and hence, must be avoided through careful engine design and operation. To smooth out the rate of pressure rise and control the ignition-timing, mixture stratification including temperature and composition inhomogeneities has been proposed.

A DNS study of ignition of a lean n-heptane/air mixture with different mean and root-mean-square(RMS) of temperature under HCCI condition revealed that when the mean temperature lies within the NTC regime, temperature fluctuation retards ove rall HCCI combustion, while it enhances the over all combustion when the mean temperatureis sufficiently greater than the temperature in the NTC regime.

In addition to temperature inhomogeneities, spark-assisted compression ignition(SACI) combustion has been proposed as one of the remedies to control the ignition timing and the pressure rise rate. In our recent DNS study, it is found that SACI combustion can control the ignition timing more precisely than HCCI combustion with temperatureinhomogeneities. Furthermore, compared to HCCI combustion, high turbulent intensity in the SACI condition significantly enhances the overall combustion by inducing many deflagration waves during the early stage of ignition as shown in Fig. 5.

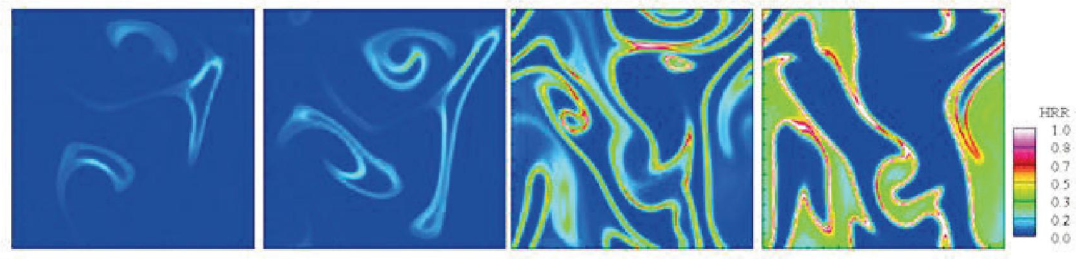

Figure 5. Isocontorus of heat release rate with high turbulent intensity. Time increases from left to right.

3. Flame instability

The diffusive-thermal instability of opposed tubular nonpremixed flames is being studied using high fidelity numerical simulations.By assuming that 1-step overall reaction, constant density, constant radial velocity without azimuthal direction velocity, the governing equations for tubular flame can be modeled. High-fidelity numerical simulations of 2-D tubular flames have been performed using the 1-D steady tubular flame solutions as the initial conditions. Figure 6compares the experimental and numerical results showing how many the flame cells form with different Damköhler numbers. The flame cells are generated due to diffusive-thermal instability (Le_F 〈 1) of the flames and hence, flame cells are able to survive much lower Damköhler numbers which 1D steady tubular flames cannot survive. The relation between the number of cells, flame location, and Damköhler number is now under investigation.

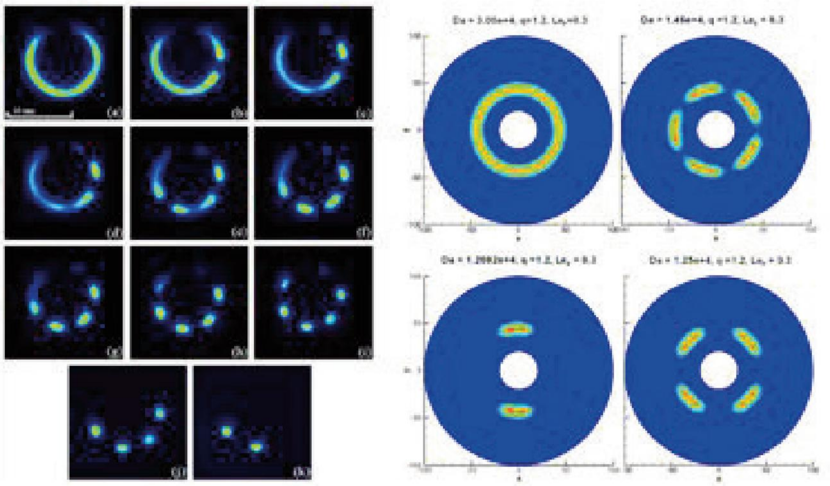

Figure 6. Comparison of experimental (left) and numerical (right) results with different Damköhler numbers

As a final remark, not only for turbulent combustion but for laminar flames, the high-fidelity numerical simulations are needed to correctly appreciate transient flame-chemistry interactions occurring in flame extinction, ignition, and instability. In the future, DNS of turbulent combustion will incorporate more complex chemistry of large hydrocarbon fuels and more complicated geometry of combustors to simulate more realistic combustion. In addition, the capability of solving multi-physics problems such as spray, two-phase flow, supercritical flow, catalytic reaction, and high Mach number flow will be utilized in DNS.