RCCI 조건에서의 혼합층을 지닌 희박 PRF/공기 혼합물의 점화특성에 관한 직접수치모사 연구

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A DNS Study of Ignition Characteristics of a Lean PRF/Air Mixture with Mixing Layer under RCCI Conditions

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ABSTRACT

The ignition characteristics of a lean PRF/air mixture with a mixing layer under reactivity controlled compression ignition (RCCI) conditions are investigated using 2-D direct numerical simulation with a 116-species PRF reduced mechanism. To account the compression heating and expansion cooling effects by piston motion, the compression heating/cooling model is adopted. For RCCI combustion, *iso*-octane and *n*-heptane are chosen as two different fuels which have low and high reactivity, respectively. The effect of the mixing layer developed by direct injection on the ignition is investigated. It is found that the first low temperature combustion, 1st stage ignition, occurs at the mixing layer, and it becomes flame and propagate into richer mixture fraction. The high temperature ignition kernels formed at *n*-heptane region and rapidly expanded toward both leaner and richer mixture fraction regions. The flame continued moving into leaner mixtures and, finally, the end-gas autoignition occurs. From the results, it is found that the mixing layer affects the development of low temperature combustion and subsequently the high temperature combustion.

Key Words : DNS, HCCI, RCCI, Mixing layer, PRF reduced mechanism

In recent decades, numerous experimental and numerical researches on next generation engines have been performed. This is because the conventional IC engines emit air pollutants such as NOx and soot. Therefore, it is necessary to develop a novel engine that can resolve the pollution issues. As one of new-generation engines, homogeneous-charge compression ignition (HCCI) engines have been spotlighted. The HCCI engine as one of low temperature combustion (LTC) engines uses highly diluted, lean, well-mixed fuel/air mixture and operates under a high compression ratio to achieve a higher thermal efficiency. Accordingly, the HCCI engine can provide high thermal efficiency like diesel engine and significantly reduce pollutant emissions without

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high price after-treatment.

Although the HCCI engine has many advantages over conventional IC engines, it still has problems for commercialization. There are two major reasons: excessive pressure rise rate (PRR) and difficulty in ignition-timing control. Since the HCCI engine uses a well-mixed fuel/air charge, the ignition delays of in-cylinder mixture are almost the same. This leads to simultaneous auto-ignition, resulting in the excessive PRR. Moreover, the HCCI engine has no direct method to control ignition timing such as spark plug or fuel injection, and hence, HCCI combustion starts only by compression heating due to the piston motion. Therefore, the chemical kinetics of the fuel/air mixture governs the overall ignition timing of HCCI combustion. Various in-cylinder conditions such as pressure, temperature, fuel composition, reactivity, and equivalence ratio can affect chemical kinetics.

To resolve the excessive PRR due to

simultaneous auto-ignition, various methods have been proposed. One of the most effective way is to induce sequential ignition of the in-cylinder charge. Unlike simultaneous auto-ignition which occurs in homogeneous mixture, sequential ignition can be obtained by introducing temperature or mixture inhomogeneities in the charge. Based on sequential ignition, HCCI variants such as spark-assisted compression ignition (SACI), stratified-charge compression ignition (SCCI), and direct dual fuel stratification (DDFS) combustion have been investigated. Among these HCCI-type combustions, reactivity controlled compression ignition (RCCI) combustion is found to control the ignition timing and combustion duration more effectively [1]

In our previous studies [2-4], the ignition characteristics of RCCI combustion under constant volume condition have been investigated. In these studies, we assumed that all the in-cylinder injections are finished and injected fuel/air mixture is well mixed prior to the top dead center (TDC) and hence, we can specify the initial conditions as the in-cylinder parameters at the TDC. Using such a method, simulation time can be shortened and fundamental ignition mechanism can be elucidated. However, the ignition characteristics during injection or right after injection are not well understood. In general, directly-injected fuel and in-cylinder fuel/air mixture form a mixing layer in between. This mixing layer affects the whole ignition process. However, the effects of the mixing layer on the HCCI combustion have not been fully understood. Recently, Krisman et al. [5-6] numerically investigated the combustion characteristics of diesel-relevant conditions in which an initial mixing layer exists between DME fuel and air. It was found that low temperature combustion significantly affects high temperature combustion and the ignition occurs as a multi-stage and multi-mode process.

Therefore, the objective of this study is to investigate the effects of mixing layer between two fuels which have different reactivity on the ignition characteristics of in-cylinder combustion under RCCI conditions using 2-D

DNSs by focusing two points: (1) the mixing layer effects, and (2) the relationship between low temperature combustion (LTC) and high temperature combustion (HTC).
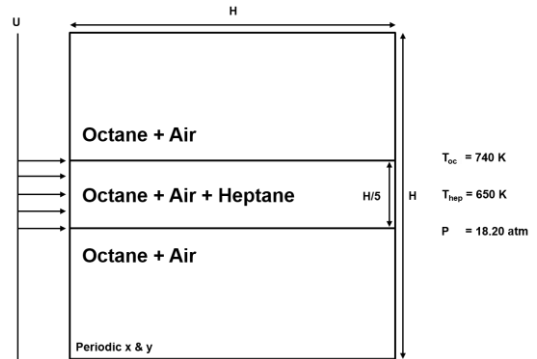

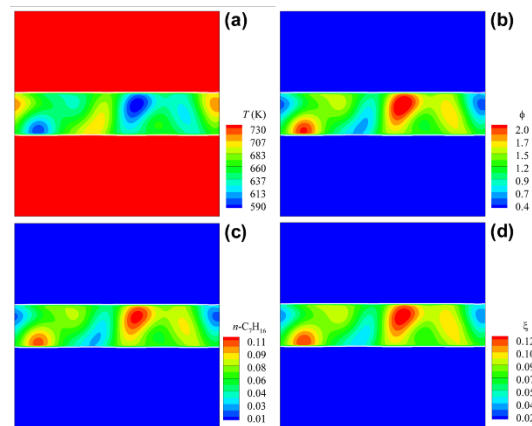**Fig. 1** Schematic diagram of the domain configuration with the boundary and initial conditions

Fig. 2 Initial temperature, ϕ, *iso*-octane and n-heptane mass fraction at shear velocity

The Sandia DNS code, S3D, was used to solve the, continuity, compressible Navier-Stokes, species continuity, and total energy equations for the ignition of PRF/air mixture. Periodic boundary conditions were imposed in all directions. To account for the compression heating and expansion cooling effects by piston motion, we include a mass source term in the governing equations as in [7].

A 116-species PRF/air reduced mechanism was adopted [8]. For all DNSs, the initial pressure and mean temperature is 18.2 atm and 720 K, respectively. The mean fuel is PRF50 (50% of *iso*-octane and 50% of *n*-heptane). For

RCCI condition, *iso*-octane and air are distributed homogeneously on the whole domain. To impose the mixing layer, *n*-heptane used directly injected fuel and set isolated center area. The temperature of *iso*-octane/air mixture is 740 K and mean temperature of *n*-heptane is 590 K and the temperature fluctuation, T', is 20 K. Figure 1 shows a schematic of the domain with initial and boundary conditions. Due to evaporative cooling of directly injected fuel, negatively-correlated (NC) $T - \phi$ distribution can exist at the *n*-heptane fuel. From a previous experimental study [9], the range of ϕ is found to be about 0.2–2.0. Similar ϕ range is introduced in the simulations. Figure 1 shows the initial temperature, ϕ, and fuel mass fraction field.

A square box of 3.2 × 3.2 mm^2 discretized with 1280 grid points in each direction was used for all 2-D DNSs. The mixing layer has σ = 50 μm thickness and the initial mixing layer is described by:

$$y(y) = \frac{1}{2}\left(\tanh\left(\frac{y - \frac{2}{5}(y_{max} - y_{min})}{\sigma} \right) - \tanh\left(\frac{y - \frac{3}{5}(y_{max} - y_{min})}{\sigma} \right) \right)$$

This specify the *iso*-octane and *n*-heptane mass fraction, y, field. The temperature field is also defined in the same way. A grid resolution of 1.25 μm is required to resolve thin flame fronts. The thinnest flame in 2-D DNSs are resolved with at least 10 grid points. Figure 2 shows the initial conditions of 2-D DNS and the scheme

Figure 3 shows the instantaneous isocontours of HRR field at the non-dimensional time, $t^* = t/t_{CA25}$, where t is the physical time and t_{CA25} is 3.20 ms. The HRR normalized by 100 J/mm^{3}s. The white solid line represents the boundary of *n*-heptane stream, in other words, mixing layer. For defining location of mixing layer, the point which has mean mixture fraction value obtained across the mixing layer is selected. The mixing layer mixture fraction equal to 0.02823. This line perfectly envelopes the injected *n*-heptane
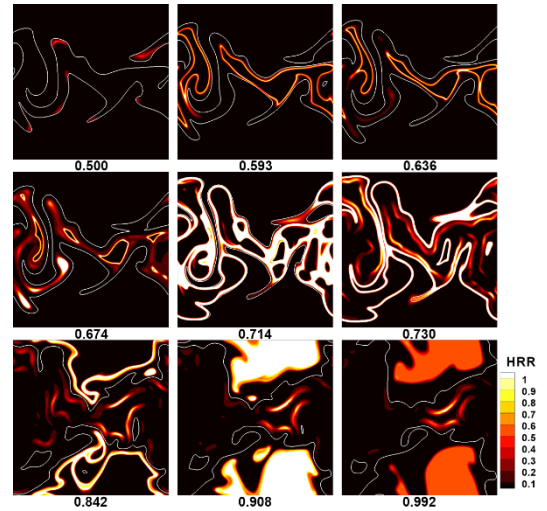
area (not shown here).

Fig. 3 Contours of normalized HRR at each normalized time, t^* ($t^* = t/t_{CA25}$)
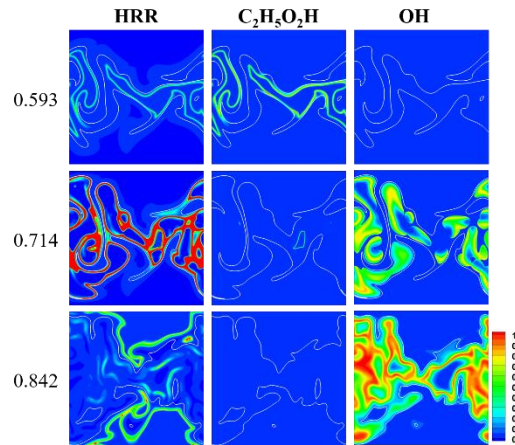

Fig. 4 Contours of normalized HRR and key species mass fractions of LTC and HTC at t^*=0.593, 0.714 and 0.842

At t^*=0.5, multiple low temperature ignition kernels occur at the mixing layer (relatively-fuel-rich region). At t^*=0.593, kernels evolve into low temperature flames which propagate into relatively-fuel-rich mixtures (into the inside of *n*-heptane stream). The low temperature flame continued moving into *n*-heptane. At a later time, low temperature flame is merged with the other flame. Moreover, low temperature flame edges occur and propagate relatively faster than flame. By t^*=0.680, the first high temperature ignition kernels form in

the n-heptane stream. These kernels form at richer mixtures than those of low temperature kernels. After this time, multiple high temperature ignition kernels form at several regions and develop into high temperature flames. Then, the kernels rapidly expand to leaner mixtures. To consume the remaining n-heptane, high temperature flame also expand toward richer mixtures. At $t^* = 0.733$, the flames burn the n-heptane mixtures and continue moving to iso-octane mixtures. The mean temperature of iso-octane mixture is around 1100 K (not shown here). However, n-heptane stream mean temperature is 2500 K. Thus, when the HTC flame crosses the mixing layer, flame undergoes excessive temperature drop. At $t^* = 0.908$, the remaining mixtures auto-ignite simultaneously, similar to the end-gas autoignition in the general HCCI engine.

In order to distinguish the effect of low- and high-temperature chemistry on flame, $C_2H_5O_2H$ and OH species are selected as a key species. $C_2H_5O_2H$ species is a short-lived intermediate species and has a peak value which is correlated with maximum HRR of 1st stage ignition. Since $C_2H_5O_2H$ lives only low temperature region, it can identify LTC well. The role of OH species is same as $C_2H_5O_2H$. However, OH is produced by HTC only, so it can identify HTC well. Figure 4 shows the instantaneous isocontour of HRR field and key species mass fractions of LTC and HTC. Each species normalized by maximum mass fraction value, 0.00042 and 0.0054, respectively. At $t^*=0.593$, $C_2H_5O_2H$ is produced along the HRR. This means that low temperature chemistry is lead the combustion. At $t^*=0.714$, both LTC and HTC key species are produced. The LTC still ongoing to consume the remaining n-heptane and the HTC occurs at overall regime of n-heptane stream. After this time, at $t^* = 0.842$, LTC is vanished and HTC flame propagate into the iso-octane mixture. In this regime, since the mean temperature is around 1200 K, HTC key species, OH, is not produced

In summary, the characteristics of ignition of a lean PRF/air mixture with mixing layer under RCCI condition are well understood.

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