HCCI 조건에 일어나는 희박 PRF/공기 혼합물의 점화특성에 관한 직접수치모사 연구

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A DNS Study of Ignition Characteristics of Lean PRF/Air Mixtures under HCCI Conditions

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ABSTRACT

Direct numerical simulations (DNSs) of ignition of lean primary reference fuel (PRF)/air mixtures under homogeneous charge compression ignition (HCCI) conditions are performed using 116-species reduced chemistry. The influence of variations in the initial temperature field, imposed by changing the variance of temperature, and the fuel composition on ignition of lean PRF/air mixtures is studied using the displacement speed analysis.

Key Words : DNS, HCCI, RPF Reduced Mechanism, Deflagration, Spontaneous ignition

1. Introduction

Homogeneous charge compression ignition (HCCI) has emerged as one of the most effective and feasible engine concept with great potential to obtain both high diesel-like efficiency and significantly reduced specific fuel consumption with ultra-low NO_x and soot emissions. However, its operating range is rather limited and there still exist difficulties in controling ignition timing and alleviating excessive pressure rise rate under a wide range of load conditions [1, 2].

By the help of the chemical mechanism reduction techniques and the development of high performance computing (HPC) clusters, however, multi-dimensional direct numerical simulations (DNSs) of HCCI combustion of hydrocarbon fuel/air mixtures can now be simulated with realistic kinetic mechanisms and provide detailed understanding of the HCCI combustion. Chen and co-workers elucidated the effect of temperature inhomogeneities and turbulent timescale on the ignition characteristics of lean hydrogen/air mixtures under HCCI conditions [3,4]. Bansal and Im [5] investigated the effects of composition inhomogeneities together with temperature fluctuations on the HCCI combustion of the same lean hydrogen/air mixture. Yoo et al. [6] investigated the ignition characteristics of lean *n*-heptane/air mixtures with different mean and root-mean-square (RMS) of temperature and the effect of the negative-temperature coefficient (NTC) regime on the overall HCCI combustion. Recently, Yoo et al. [7] studied the ignition characteristics of a lean *iso*-octane/air mixture with temperature fluctuations and spark-ignition timing under both HCCI and spark-assisted compression ignition (SACI) conditions.

Up to now, most of the previous DNS studies were focused on the effects of thermal and composition stratifications and turbulence timescales on HCCI combustion. Therefore, the objective of the present study is to understand and compare the ignition characteristics of different hydrocarbon fuel/air mixtures under HCCI conditions. For this purpose, primary reference fuels (PRFs) are chosen because they have widely been used to investigate the combustion characteristics of HCCI engines by the engine community.

PRF is a fuel mixture of *n*-heptane and

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iso-octane. For instance, PRF100 and PRF50 represent 100 % of *iso*-octane, and 50 % *iso*-octane plus 50 % *n*-heptane by volume, respectively. Ultimately, the present study aims to provide strategies to control the rate of heat release in HCCI combustion by performing two-dimensional parametric DNSs, systematically varying two key parameters: 1) the fuel composition and 2) the initial variance of the temperature, T'.

2. Numerical methods and initial conditions

For the present DNS study, the Sandia DNS code, S3D, was used with the 116-species PRF/air reduced chemistry linked with CHEMKIN and TRANSPORT software libraries for evaluating reaction rates and thermodynamic and mixture-averaged transport properties. As in the previous DNS studies of hydrocarbon fuel/air HCCI combustion [5,6], periodic boundary conditions were imposed in all directions such that ignitions of PRFs/air mixtures occur at constant volume.

The initial uniform equivalence ratio, ϕ and pressure, p, are 0.3 and 20 atm, respectively. Note that $\phi = 0.3$ is adopted to elucidate the ignition characteristics of a PRF/air mixture under high load conditions. A total of nine different DNS cases were performed in the parameter space of initial physical conditions: different fuels (PRF50, PRF80, and PRF100); and temperature fluctuation root mean square, T'. Details of the physical and numerical parameters for the nine cases are presented in Table 1.

The computational domain is a 2-D square box with each domain size, L, of 3.2 mm, discretized with N = 640 grid points.

3. Results and discussion

Nine DNS cases were performed to elucidate the effect of temperature fluctuations on the ignition characteristics of the different PRFs/air mixtures. Three different degrees of temperature fluctuation are chosen: T' = 15, 30, and 60 K. Figure 1 shows the temporal evolution of the mean pressure, $\bar{p}$, and the mean heat release rate, $\bar{\dot{q}}$. To show the reference for the 2-D cases, the corresponding 0-D cases are also added in the figure.

Table 1 Physical parameters of the DNS

Case	Fuel	T_0(K)	T' (K)	τ_t(ms)	τ_{ig}^0(ms)
1	PRF100	1024	15	2.5	2.50
2	PRF100	1024	30	2.5	2.50
3	PRF100	1024	60	2.5	2.50
4	PRF80	1024	15	2.5	2.39
5	PRF80	1024	30	2.5	2.39
6	PRF80	1024	60	2.5	2.39
7	PRF50	1024	15	2.5	2.29
8	PRF50	1024	30	2.5	2.29
9	PRF50	1024	60	2.5	2.29

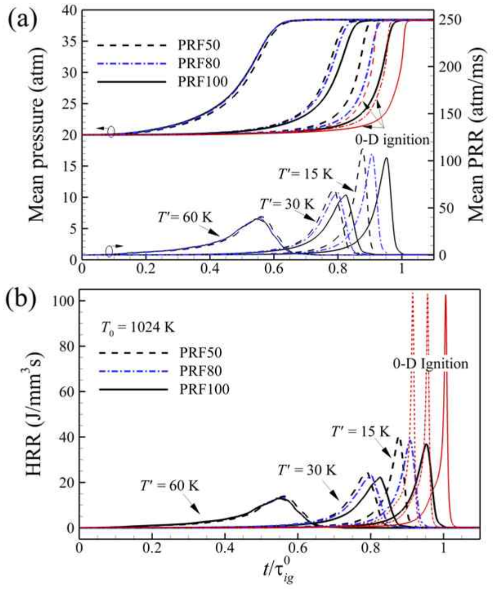

Fig. 1 Temporal evolution of (a) mean pressure and heat release rate for 2-D cases and (b) heat release rate for 0-D cases.

As shown in the figure, the mean pressure increases more slowly and heat release rate (HRR) becomes smother with increasing T' regardless of the fuel composition. These results are qualitatively identical to those of ignition characteristics of the hydrogen/air, *n*-heptane/air, and *iso*-octane air mixtures with high mean initial temperature [3~7].

For cases with small T' (cases 1~3), τ_{ig} increases with increasing *iso*-octane volume percent in the PRF (PRF50 → 80 → 100). For small T', the overall combustion occurs primarily through spontaneous ignition and hence, the ignition characteristics of 2-D

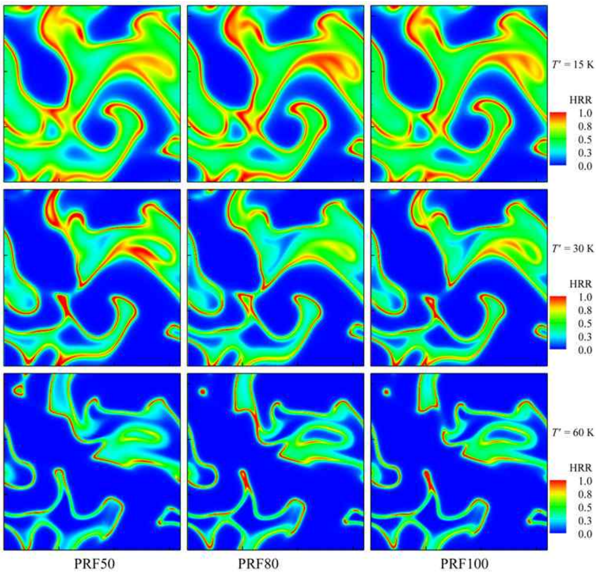

Fig. 2 Isocontours of normalized HRR (from left to right, RPF50, RPF80 and PRF 100 at t/τ_{ig} = 0.88, 0.91, and 0.95 with T' = 15 K (top); t/τ_{ig} = 0.79, 0.80, and 0.82 with T' = 30 K (middle); t/τ_{ig} = 0.62, 0.59, and 0.59 with T' = 60 K (bottom).

cases becomes similar to those of 0-D homogeneous auto-ignition, which is readily verified from Fig. 2. As shown in the figure, for small T' cases, HRR occurs in almost the whole domain simultaneously. For large T' cases, however, HRR occurs largely in thin sheets, although relatively low HRR also occurs over a broader area.

For cases with large T' (cases 7~9), however, the temporal evolutions of $\overline{\dot{q}}$ are almost identical for the three cases, implying that the effect of different fuel compositions of PRFs on combustion is negligible. As seen in Fig. 2, the combustion in large T' cases occurs through the mixed mode of deflagration and spontaneous ignition. Therefore, the characteristics of flame propagation, or the turbulent flame speed is supposed to determine the overall combustion.

In the present study, an identical initial turbulence field is used for all 2-D DNSs and hence, only the laminar flame speed can effectively change the turbulent flame speed. Note that the laminar flame speeds of different PRFs in the present study are nearly identical. As such, the combustion phase of the three cases would be the same only if the initial ignition kernels are not affected significantly by the turbulence field.

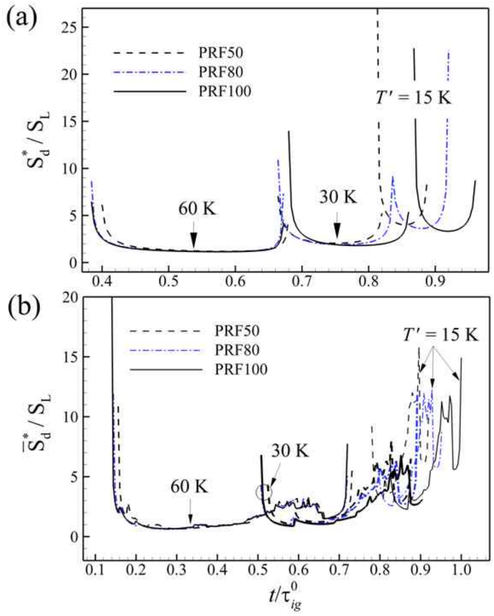

Fig. 3 Temporal evolution of (a) S_d^* for one-dimensional reference cases (b) the mean front speed, $\overline{S_d^*}$, for two-dimensional DNS cases with T' = 15, 30, and 60 K, and different PRFs

The result from large T' cases implies that as the deflagration mode of combustion is predominant, the effect of different fuel composition or chemistry of PRF/air mixtures on the ignition characteristics can be neglected. This may justify that HCCI engines can operate on various types of fuels with appropriate methods in controling ignition timing and the spread of HRR.

To qualitatively distinguish between spontaneous ignition and deflagration mode of combustion, the density-weighted displacement speed, S_d^* is adopted to delineate between two combustion modes.

Figure 3 shows the temporal evolution of (a) S_d^* for 1-D reference cases (b) the mean front speed, $\overline{S_d^*}$, for 2-D DNS cases, all of which are normalized by the corresponding laminar flame speed, S_L, found to be approximately 0.385, 0.37, and 0.368 m/s for PRF50, PRF80 and PRF100, respectively. It is readily observed from Fig. 3 that the mean front speeds exhibit a characteristic 'U' shape qualitatively consistent with previous studies [6,7]. The occurrence of the 'U'-shaped mean front speed is attributed to the initial thermal run-away in the nascent ignition kernel during the early phase of combustion and the burnout of remaining charge due to compression heating during the last phase of combustion [6,7].

The overall combustion is advanced with increasing T', but retarded for cases with small T'. Note also that, deflagration of relatively constant speed is predominant for cases with large T' , and hence, flame speed exhibits values close to S_L with increasing T'. Figure 3 also reveals that the duration of the region of constant speed at the bottom of the 'U' shape increases with increasing T', proposing that combustion at the reaction waves occurs primarily by deflagration rather than by spontaneous ignition. On the contrary, for cases with small T', the front speed is much greater than S_L. These results indicate that a small degree of thermal stratification leads an excessive rate of heat release due to simultaneous auto-ignition occurring throughout the whole domain, which should be avoided in HCCI combustion. For large T', however, deflagration mode of combustion occurs sooner and persist longer than the corresponding 1-D cases because the large T' induces more locally hotter mixtures than those the 1-D cases, and hence, locally auto-ignition can occur and develop into a deflagration wave sooner than in the 1-D cases.

These results also suggest that the critical degree of thermal stratification for smooth operation of HCCI engines depends largely on the temperature fluctuation, T', such that the effects of different chemical compositions in fuels are hence reduced. On that account, it is crucial to consider the role of the temperature fluctuation, T', to ensure a moderate pressure rise rate.

4. Concluding remarks

The effects of thermal stratification and fuel composition on auto-ignition of lean PRF/air mixtures under HCCI conditions are investigated using DNS with a 116-species reduced mechanism for PRF/air mixture. The nine 2-D DNSs were carried out with different degrees of temperature fluctuations and PRFs. The results show that, in general, larger T' induces greater temporal spreading of the mean HRR due to the predominance of deflagration mode and hence, the physical properties (flame speed) rather than chemistry of the fuel are more important in determining the combustion characteristics. On the contrary, spontaneous ignition mode prevails for small T' such that the effect of fuel compositions or chemistry on the overall ignition are more important than the physical properties of the fuel/air mixtures.

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