고압·중간 온도 조건에서의 희박 PRF/공기 혼합물 점화에 관한 직접수치모사 연구

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A DNS study of ignition of lean PRF/air mixture under high pressure and intermediate temperature condition

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ABSTRACT

Two-dimensional direct numerical simulations (DNSs) of the ignition of lean primary reference fuel (PRF)/air mixtures at high pressure and intermediate temperature near negative temperature coefficient (NTC) regime were performed to elucidate the effects of fuel composition, thermal stratification, and turbulence on PRF homogeneous charge compression-ignition (HCCI) combustion. In general, it was found that the mean heat release rate increases slowly and the overall combustion occurs fast with increasing thermal stratification regardless of the fuel composition. In addition, the effect of the fuel composition on the ignition characteristics of PRF/air mixtures was found to be significantly reduced with increasing thermal stratification. The reduction of the fuel effect under the high degree of thermal stratification is caused by the nearly identical propagation characteristics of deflagrations of different PRF/air mixtures. Ignition Damköhler number is proposed to quantify the successful development of deflagrations from nascent ignition kernels. It was verified that for cases with large ignition Damköhler number, turbulence with high intensity and short-timescale can advance the overall combustion by increasing turbulent flame area instead of homogenizing initial mixture inhomogeneities.

Key Words : HCCI, DNS, primary reference fuel (PRF), thermal stratification.

The fundamental ignition characteristics of various fuel/air mixtures under lean, dilute, elevated pressure and relatively low temperature have been widely investigated due to their practical relevance to homogeneous charge compression-ignition (HCCI) engine combustion [1-13].

HCCI engines have no explicit ignition method such that ignition timing in HCCI combustion is primarily governed by the chemical kinetics of fuel/air mixture, which depend highly on overall mixture composition, temperature, and pressure. There have been a lot of attempts to control the ignition timing and alleviate the excessive pressure rise rate (PRR) by applying to HCCI engines different fuel injection strategies, fuel preparation, and thermal management including exhaust gas recirculation (EGR) [1-3].

In many previous DNS studies [4-6, 10, 13], the ignition characteristics of hydrogen/air mixtures exhibiting only one-stage ignition were investigated and as such, the effect of negative-temperature coefficient (NTC) regime on HCCI combustion was not appreciated. The NTC regime usually appears as a result of the low-temperature oxidation of large hydrocarbon fuels exhibiting two-stage ignition. The effect of NTC regime on HCCI combustion was first investigated by Yoo et al. [7].

It is of interest to note that in our previous DNS study of the ignition of PRF/air mixtures at elevated pressure and high temperature [9], it was found that the effect of different fuel

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composition on the overall combustion vanishes with increasing temperature inhomogeneities. However, the homogeneous ignition delays of different PRF/air mixtures under high pressure and intermediate temperature conditions, which are more relevant to practical HCCI combustion, show a big disparity among the mixtures (see Fig. 1), and hence, it may be expected that the effect of fuel composition

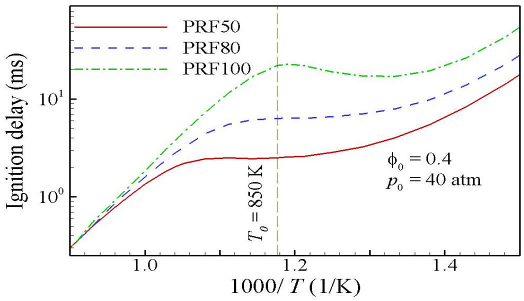

Fig. 1 0-D ignition delays as a function of initial temperature for different PRF/air mixtures at p_0 = 40 atm and of ϕ_0= 0.4.

would not vanish even with large temperature fluctuation. Moreover, the early phase of ignition of a fuel/air mixture with very large temperature fluctuation may not be affected by turbulence [8]. The objective of the present study is to understand and compare the ignition characteristics of different fuels at high pressure and near the NTC regime by varying three key parameters: 1) the fuel composition, 2) the initial temperature fluctuation, and 3) the initial turbulence intensity. Note that PRF is a fuel mixture of pure *n*-heptane and *iso*-octane; for instance, PRF80 is comprised of 80% iso-octane and 20% *n*-heptane by volume.

For the present DNSs, the Sandia DNS code, S3D, was used with a 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 [7-9], periodic boundary conditions were imposed in all directions such that ignitions of PRF/air mixtures occur at a constant volume.

For all simulations, the initial mean temperature, T_0 was 850 K, the initial uniform equivalence ratio ϕ_0 is 0.4 and the pressure p_0 is 40 atm. Note that p_0 of 40 atm was adopted to elucidate the ignition characteristics of PRF/air mixtures under high pressure similar to that in HCCI engines. Ten different DNSs were performed in the parameter space of the initial physical conditions: different fuel compositions; temperature fluctuation RMS T'; and turbulence velocity fluctuation u'. Henceforth, τ_{ig} represents the time at which the maximum mean heat release rate (HRR) occurs for all 0-D, 1-D, and 2-D simulations. The superscript 0 corresponds to the 0-D simulation at a constant volume. For PRF50

Table. 1 Physical and numerical parameters of the DNS

Case	Fuel	T' (K)	τ_t (ms)	u' (m/s)
1	PRF50	15	2.5	0.5
2	PRF50	60	2.5	0.5
3	PRF50	120	2.5	0.5
4	PRF80	15	2.5	0.5
5	PRF80	60	2.5	0.5
6	PRF80	120	2.5	0.5
7	PRF50	60	0.5	2.5
8	PRF50	120	0.5	2.5
9	PRF80	60	0.5	2.5
10	PRF80	120	0.5	2.5

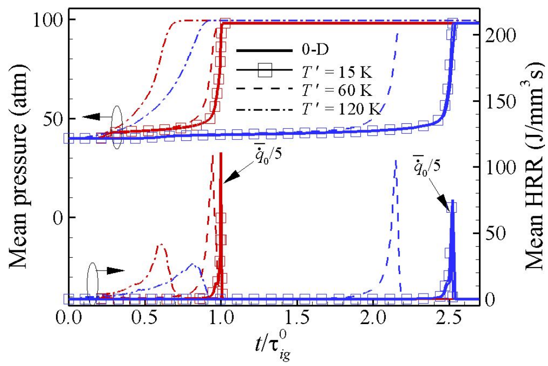

Fig. 2 Temporal evolutions of the mean pressure and mean HRR for Cases 1~6. Red and blue lines represent, respectively, PRF50 and PRF80.

τ^0_{ig}=2.5 ms and PRF80 τ^0_{ig}=6.3 ms. Details of the physical parameters are in Table 1. The computational domain is a 2-D square box with each domain size, L, of 3.2 mm, discretized with N=1280 for T'=120 K, otherwise, 640 grid points. In the first parametric study, six different DNS cases

(Cases 1~6) were simulated (see Table 1) to elucidate the combined effect of the initial fuel composition and temperature fluctuation on the ignition of the fuel/air.

Figure 2 shows several ignition characteristics of the PRF/air mixtures. noted that the 0-D ignition delay of the PRF50/air mixture (τ_{ig}^{0} = 2.5 ms) was chosen as the reference time.

First, $\bar{p}$ increases more slowly and $\bar{\dot{q}}$ is more distributed over time with increasing T' for all fuel compositions. In addition, the shape of the overall combustion for Cases 1 and 4 with small T' are nearly identical to the corresponding 0-D ignition. The PRF50/air and PRF80/air mixtures exhibit nearly constant ignition delays at intermediate temperatures around 850 K as shown in Fig. 1, implying that the mixtures with small T' cannot take any advantage of temperature fluctuations to advance the overall combustion [7, 9].

Second, the overall combustion occurs fast and the peak $\bar{\dot{q}}$ is reduced with increasing T' for the same PRF/air mixture, which results in the elongation of vigorous combustion phase. This is primarily attributed to the occurrence of deflagrations in the HCCI combustion by large degree of T', leading to the spread of $\bar{\dot{q}}$ and the fast occurrence of the overall combustion. Large T' generally induces the mixed mode of combustion of deflagration and spontaneous auto-ignition while small T' leads to the spontaneous auto-ignition throughout the whole domain.

Third, for the cases with the same T', the effect of fuel composition is significantly reduced with increasing T'. For cases with small T' (Cases 1 and 4), τ_{ig} increases significantly with increasing *iso*-octane volume percentage in the PRF as can be expected from their τ_{ig}^{0}. However, for cases with large T' (Cases 3, 6), the difference between τ_{ig} of the PRF/air mixtures is significantly decreased. This result implies that the effect of different fuel compositions of PRFs on HCCI combustion may vanish with increasing T'.As found in previous studies [4-9], the deflagration mode of combustion can be dominant for the cases with large T' and, hence, the propagation characteristics of each PRF/air deflagration wave become more important than those of the chemical kinetics for initiating nascent ignition kernels.

In most previous DNS studies of HCCI combustion [5-9], it was found that turbulence with short τ_t and large u' tends to homogenize initial temperature inhomogeneities of fuel/air mixture more than that with long τ_t and small u', and as such, the overall combustion is retarded while occurring by spontaneous ignition. However, it was also found from [8] that turbulence with short τ_t and large u' can advance the overall combustion by increasing the area of turbulent deflagrations.

Four additional DNSs (Cases 7~10) were performed with greater u' to elucidate the effect of turbulence. Fig. 3 shows the effect of turbulence (u'=0.5 m/s and 2.5 m/s). For cases with T' of 60 K, which is relatively small considering that it induces a small range of ignition delays of the initial mixture, turbulence with short τ_t and large u' can effectively homogenize the mixtures and hence, both τ_{ig} and the peak of $\bar{\dot{q}}$ are increased and the overall combustion is more apt to occur by

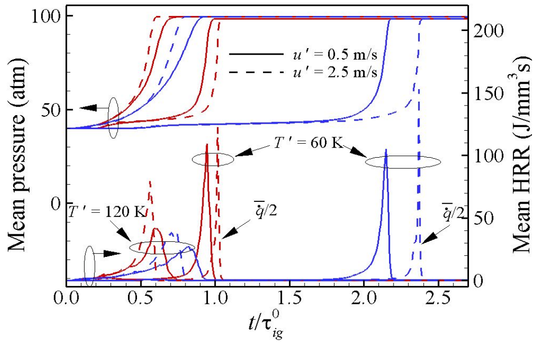

Fig. 3 Temporal evolutions of the mean pressure and mean HRR for Cases 2, 3, and 5 ~10. Red and blue lines represent, respectively, PRF50 and PRF80.

Table. 2 Da_{ig} for PRF50 cases

Case	u' (m/s)	Da_{ig}
2	0.5	2.17
8	2.5	0.43
3	0.5	25
9	2.5	5.0

spontaneous ignition for both RPF/air mixtures. For cases with relatively large T' of 120 K, however, τ_{ig} is reduced and the peak of $\bar{\dot{q}}$ is increased with increasing u', which seems to be opposite to the cases with small T' and what was found in previous studies [5-9].

To quantify the effect of turbulence on the early ignition characteristics, we introduce an ignition Damköhler number, Da_{ig}, which evaluates the overall competition between ignition and turbulence dissipation during the early phase of HCCI combustion: $Da_{ig} \equiv \tau_t / \tau_{ig,10\%}$, where $\tau_{ig,10\%}$ is the lowest 10% ignition delay of the initial mixture, which represents the ignition time-scale of the hottest mixtures. If $Da_{ig} \gg O(1)$, the occurrence of nascent ignition kernels and their evolution to deflagrations are nearly independent of turbulence. On the contrary, if $Da_{ig} \ll O(1)$, the homogenization of the initial mixture by turbulence can completely be finished much earlier than the corresponding 0-D ignition delay and as such, the overall combustion becomes much more like the 0-D ignition.

Table 2 shows value of Da_{ig} for PRF50 cases. For cases 2 and 8, as high u' $Da_{ig} \ll O(1)$ that means, they are highly depend on turbulence; consequently, the overall combustion is retarded as shown in Fig. 3.

For Cases 3 and 9 (T' = 120 K), however, $Da_{ig} \gg O(1)$ such that the early phase of ignition becomes nearly independent of turbulence. Once deflagrations are developed from the ignition kernels, their evolutions can be highly affected by local turbulence, such that large u' is more likely to advance the overall combustion by increasing turbulent flame area. Fig. 4 shows the instantaneous snap shots of isocontour of HRR for Cases 3 and Case 9, which readily identify the increase of turbulent flame area by large u'.

The effects of PRF composition, T', and u' on the ignition of lean PRF/air mixtures at high pressure and intermediate temperature are investigated by 2-D DNSs. larger T' induces spreading of the mean HRR regardless of PRF composition because the deflagration mode is predominant at the reaction fronts for large T'. However, spontaneous ignition prevails for small T' and, hence, simultaneous auto-ignition occurs throughout the whole domain, resulting in an excessive HRR The effect of fuel composition on the ignition of PRF/air mixtures is found to be significantly reduced with increasing T' because the deflagration mode prevails at the reaction fronts and the propagation characteristics of deflagrations are nearly identical.

Da_{ig} was proposed to evaluate the effect of turbulence on the early evolution of deflagrations. Turbulence with $Da_{ig} \ll O(1)$ can effectively homogenize the mixtures and delay the occurrence of deflagrations. However, turbulence with $Da_{ig} \gg O(1)$ can advance the overall combustion by increasing turbulent flame area because the effect of turbulence on the occurrence of nascent ignition kernels and their evolution to deflagrations becomes insignificant.

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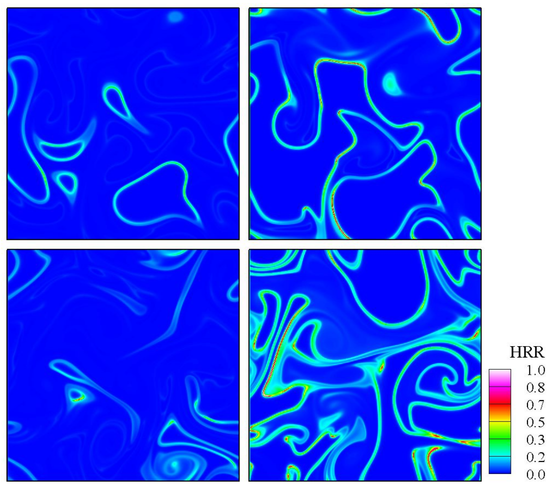

Fig. 4 Isocontours of the normalized heat release rate for Cases 3 (top) and 9 (bottom). From left to right, t/τ_{ig}^0 = 0.36 and 0.52, respectively.

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