불균일한 온도 및 조성을 지닌 희박 바이오디젤/공기 혼합물의 점화특성에 관한 직접수치모사 연구

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A DNS study of ignition of lean biodiesel/air mixture with temperature and composition inhomogeneities

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ABSTRACT

Two-dimensional direct numerical simulations of ignition of a biodiesel/air mixture with temperature (T) and equivalence ratio (ϕ) stratifications are investigated using a 73-speices reduced chemistry. This study aims at three case studies (1) baseline cases with either only thermal stratification or only fuel concentration stratification; and the two highly feasible scenarios of the $T-\phi$ distribution (2) uncorrelated $T-\phi$ correlations; and (3) negatively correlated $T-\phi$ correlations. The uncorrelated $T-\phi$ distribution leads to a smooth combustion due to a mixed mode of combustion of deflagration and spontaneous ignition. The negatively-correlated $T-\phi$ distribution results in a severe occurrence of heat release rate throught the whole domain because of spontaneous ignition.

Key Words : DNS, HCCI, Biodiesel reduced mechanism, composition inhomogeneities

Homogeneous charge compression-ignition (HCCI) combustion has been extensively investigated by the engine community due to its great potential to obtain both high diesel-like efficiency and significantly reduced specific fuel consumption with ultra-low NO_x and soot emissions. However, a few challenges in the development of real HCCI engines are still remaining. One of the issues is how to control precisely the ignition timing of combustion and prevent an excessive pressure-rise rate (PRR) under high-load conditions [1,2].

As a promising remedy for controlling the ignition timing and pressure rise rate as well as extending the operating range of HCCI combustion, stratified-charge compression ignition (SCCI) combustion has been turned to [1,2]. With the help of fuel stratification, a sequential ignition event can be achieved because locally-richer mixture tends to ignite first and then ignition propagates towards nearby leaner mixture. As a result, SCCI combustion enables a smooth combustion sequence, preventing rapid heat release rate (HRR) and reducing the peak PRR. Therefore, SCCI combustion under HCCI condition has been subject to many fundamental researches [1-3]. Recently, Bansal and Im investigated the ignition characteristics of a hydrogen/air mixture with both temperature and composition inhomogeneities using two-dimensional (2-D) DNSs [3]. It was found that composition inhomogeneities together with temperature fluctuations spread out HRR further compared to temperature fluctuations only. However, the results may not be directly applicable to hydrocarbon fuel/air mixtures exhibiting two-stage ignition.

The objective of the present 2-D DNSs study, therefore, is to provide a fundamental understanding of the ignition characteristics of a ignition hydrocarbon fuel/air mixture with thermal and fuel stratifications under high

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Table 1 Physical parameters of the DNS

Case	Type	T_0 (K)	T' (K)	ϕ_0	ϕ'	τ_{ig}^0 (ms)
1	BL	850	15	0.45	–	1.0
2	BL	850	60	0.45	–	1.0
3	BL	850	–	0.45	0.05	1.0
4	BL	850	–	0.45	0.10	1.0
5	UC	850	15	0.45	0.05	1.0
6	UC	850	15	0.45	0.10	1.0
7	UC	850	60	0.45	0.05	1.0
8	UC	850	60	0.45	0.10	1.0
9	NC	850	15	0.45	0.05	1.0
10	NC	850	15	0.45	0.10	1.0
11	NC	850	60	0.45	0.05	1.0
12	NC	850	60	0.45	0.10	1.0

pressure and intermediate temperature by using biodiesel with two-stage ignition. The simulations were conducted by systematically changing two key parameters: (1) initial temperature fluctuation and (2) initial equivalence ratio fluctuation.

For the present DNS study, the Sandia DNS code, S3D, was used with a 73-species biodiesel/air reduced chemistry. 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 the biodiesel/air mixture occurs at constant volume. In the present study, the biodiesel reduced mechanism, which consists of 25% methyl decanoate (MD), 25% methyl 9-decanoate (MD9D), and 50% n-heptane by volume was adopted [4].

For all simulations, the initial mean temperature, T_0, mean equivalence ratio, ϕ_0, and the initial uniform pressure, p_0, are 850 K, 0.45, and 40 atm, respectively. A total of twelve DNSs were performed by changing two key parameters: temperature fluctuations, T', of 15 K and 60 K, and equivalence ratio fluctuations, ϕ' of 0.05 and 0.10. Details of the physical and numerical parameters for each case are listed in Table 1.

Depending on fuel delivery strategies, injection timings, amount of EGR, intake charge heating, wall heat loss etc., different $T-\phi$ distributed relations may exist at the TDC. In the present study, therefore, three distinct cases of initial $T-\phi$ correlations are elucidated: (1) baseline cases with solely either

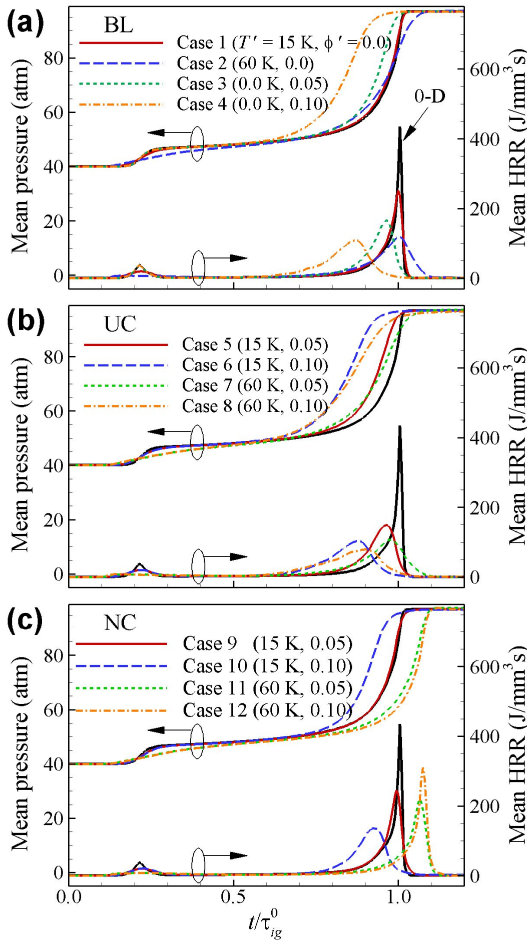

Fig. 1 Temporal evolution of mean pressure and heat release rate for (a) Cases 1-4, (b) Cases 5-8, and (c) Cases 9-12. Thick lines represent the corresponding 0-D homogeneous ignition.

temperature (Cases 1 and 2) or equivalence ratio fluctuation (Cases 3 and 4), (2) uncorrelated $T-\phi$ distribution (Cases 5−8), and (3) negatively-correlated $T-\phi$ distribution (Cases 9−12).

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

In the present study, total twelve different 2-D DNS cases were simulated: four baseline cases with T' only or ϕ' only (Cases 1−4), four cases with uncorrelated $T-\phi$ distribution (Cases 5−8), and four cases with negatively-correlated $T-\phi$ distribution (Cases 9−12) (see Table 1). Note that under the current initial temperature, equivalence ratio, and pressure condition, the low-temperature chemistry of biodiesel oxidation exists such that two-stage ignition occurs in the ignition process of the biodiesel/air mixture.

Figure 1 shows the temporal evolutions of mean pressure, $\bar{p}$, and mean heat release rate, $\bar{\dot{q}}$, for Cases 1−12. It can be found from Fig. 1 that for cases with T' only (Cases 1 and 2), $\bar{p}$ increases more slowly and $\bar{\dot{q}}$ is more spread out over time with increasing T'. This result is qualitatively consistent with previous studies [5-9]. For Case 1 with small T', however, the temporal evolutions of $\bar{p}$ and $\bar{\dot{q}}$ are almost identical to those of 0-D ignition. It is of interest to note that although high T' smooths out $\bar{p}$ and $\bar{\dot{q}}$, the maximum $\bar{\dot{q}}$ for Case 2 occurs nearly at the same time as τ_{ig}^{0} and that of Case 1.

The effect of ϕ' on the biodiesel HCCI combustion is investigated with Cases 3 and 4 (see Fig. 1a). Like the effect of T', $\bar{p}$ increases more slowly and $\bar{\dot{q}}$ is more distributed over time with increasing ϕ'. Unlike the cases with T'only, however, the overall combustion occurs quickly with increasing ϕ'. It was found from previous study that, depending on the mean temperature, thermal stratification may advance or retard the overall HCCI combustion of n-heptane/air mixture exhibiting two-stage ignition. However, composition fluctuation is more apt to advance the overall HCCI combustion in time regardless of the mean temperature and equivalence ratio in HCCI combustion. As such, these results imply that fuel stratification can be a more effective means for preventing excessive PRR and controlling ignition timing for hydrocarbon-fueled HCCI combustion.

Figure 1b shows the combined effect of T' and ϕ' on the overall HCCI combustion. Note that $T-\phi$ fields are uncorrelated. Several observations can be made from the figure. First, for small T' (Cases 5 and 6), the temporal evolutions of $\bar{p}$ and $\bar{\dot{q}}$ are nearly identical to those of the corresponding baseline cases with the same ϕ' (Cases 3 and 4). As shown in Fig. 1a, small T' has nearly no effect on the overall HCCI combustion (Case 1), and as such, the composition fluctuation has a first-order effect on the ignition characteristics of biodiesel/air mixture. Second, large T' with ϕ' (Cases 7 and 8) smooths out $\bar{\dot{q}}$ more compared to small T'(Cases 5 and 6). For these cases, large T' with ϕ' has a synergetic effect in preventing excessive PRR by spreading out $\bar{\dot{q}}$. However, large T' does not advance the overall combustion; τ_{ig} for Cases 5 and 6 are 0.87 and 0.96 ms respectively, whereas τ_{ig} for Cases 7 and 8 are 0.90 and 0.97 ms respectively. Third, the overall combustion occurs quickly with increasing ϕ', similar to the baseline cases, while the maximum $\bar{\dot{q}}$ is decreased.

Figure 1c shows the combined effect of negatively-correlated T' and ϕ' on the overall HCCI combustion, which represents one of the most probable $T-\phi$ relation achieved with late-direct injection. Note that the competitive effect of T' and ϕ' on the biodiesel HCCI combustion can be elucidated with the negatively-correlated $T-\phi$ fields. Several points are readily to be noted from the figure. First, for Case 9, the temporal evolutions of $\bar{p}$ and $\bar{\dot{q}}$ are quite similar to those of the corresponding 0-D ignition and Case 1, implying that the advancement and spread of the overall HCCI combustion caused by ϕ' (Case 3) are almost annihilated by the negative correlation of $T-\phi$ fields. Second, large ϕ' (Case 10), however, can overcome the mutual canceling effect of the negative correlation of $T-\phi$ on the overall combustion. As such, $\bar{\dot{q}}$ is more distributed over time and the overall combustion is advanced. Third, unlike Cases 9 and 10, ϕ' with large T' (Cases 11 and 12) retards the overall combustion which seems to occur by the spontaneous mode of combustion more like the corresponding 0-D ignition. This is primarily because the initial local fluctuation of composition together with T' almost always increases ignition delays.

To further identify the combustion characteristics of the 2-D DNS cases, the instantaneous HRR contours for Cases 1, 2, 8

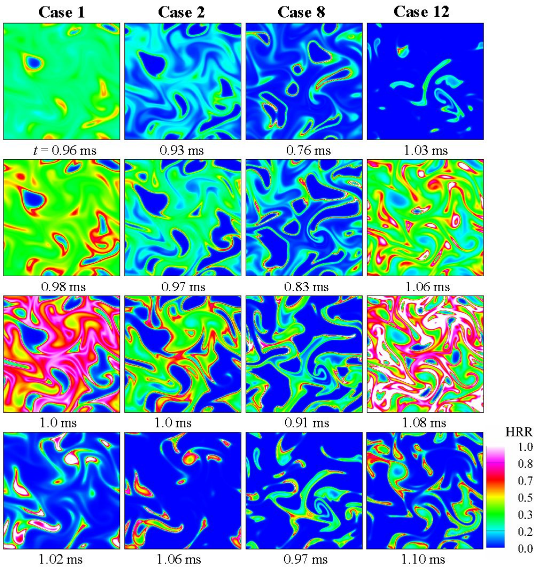

Fig. 2 Isocontours of normalized heat release rate for Cases 1, 2, 8, and 12.

and 12 are examined as shown in Fig. 2. Note that each HRR field is normalized by $\dot{q}_m^0$ = 434.5 J/㎣s which is the maximum HRR of the 0-D homogeneous ignition. It should also be noted that the third figure from the top shows the HRR field at τ_{ig}.

It is readily observed that, for Cases 1 (T' = 15 K only) and 12 (T' = 60 K, ϕ' = 0.1 with negative correlation), HRR occurs throughout the whole domain in quite short time; the duration of combustion (5% to 95% of cumulative HRR) for Cases 1 and 12 are approximately 0.12 and 0.10 ms respectively. In addition, the combustion occurs by the spontaneous auto-ignition. For Cases 2 (T'= 60 K only) and 8 (T'= 60 K, ϕ' = 0.1 with uncorrelation), however, high HRR occurs at thin sheet regions as deflagration even though low HRR happens in much broader regions, implying that mixture with large T' with/without uncorrelated ϕ may lead to a mixed mode of combustion—deflagration mode together with spontaneous ignition, thereby effectively reducing excessive HRR and advancing the overall combustion as well as elongating the duration of combustion.

The effect of thermally and compositionally stratified biodiesel/air mixtures involving the low temperature heat release region under HCCI conditions are investigated by using DNS with a 73-species reduced mechanism. Different $T-\phi$ spectrums are initially superimposed in 2D flow fields: (1) the reference cases with either solely T' or solely ϕ' stratification; (2) the uncorrelated $T-\phi$ distributions; and (3) the negatively correlated $T-\phi$ distributions. The results revealed that a stratified biodiesel/air mixture with a high levels of fuel stratification with a small T' offers a great potential of controlling the ignition timing as well as providing a smooth HCCI operation under high load conditions. However, it should deliberately introduce an appropriate stratified $T-\phi$ field such that excessive pressure rise rate can be prevented

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