DDFS 조건에서의 PRF/공기 혼합물 점화의 분사시기 효과에 대한 직접수치모사 연구

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A DNS Study of the Effects of Injection Timing on the Ignition of PRF/Air Mixture under DDFS Conditions

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ABSTRACT

The ignition characteristics of PRF/air mixtures under direct dual fuel stratification (DDFS) conditions are investigated using 2-D direct numerical simulations with a 117-species reduced PRF mechanism. The effects of compression heating and expansion cooing by the motion of piston in an engine cylinder are also accounted for by adopting a compression heating/cooling model. *iso*-Octane and *n*-heptane are selected as two different fuels of low and high reactivity, respectively, and the overall mixture reactivity is PRF70. A pseudo *iso*-octane model is developed to simulate the effects of injection timing on the DDFS combustion phasing. It is found that DDFS combustion is highly sensitive to the injection timing, t_{inj} . The combustion phasing is delayed with advancing t_{inj} , and overall combustion proceeds in a mixed mode of spontaneous ignition fronts and deflagration. As such the combustion duration is elongated in turn reducing the peak heat release rate (HRR). When *iso*-octane is delivered just near top dead center (TDC) into the undergoing-reacting charge, the overall combustion at this point occurs dominantly by auto-ignition. Its burning rate from this point, however, is primarily governed by diffusion-limited injection. As a result, the HRR is still well-controlled and entirely dependent on the timing and duration of late *iso*-octane injection.

Key Words: DNS, HCCI, RCCI, DDFS, PRF reduced mechanism

Reactivity controlled compression ignition (RCCI) combustion have demonstrated superior controllability of combustion process without sacrificing the benefits of conventional homogeneous charge compression ignition (HCCI) combustion such as high thermal efficiency with ultra-low emissions. As shown in Fig.1, RCCI combustion uses two fuels with different auto-ignition characteristics. Low-reactivity fuel is supplied through port injection to make it well mix with oxidizer, followed by one or more direct injections of high-reactivity fuel create spatially to inhomogeneities in reactivity and equivalence ratio. By adjusting the mass ratio of two fuels and the timing/duration of high-reactivity fuel

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injections, RCCI can provide a fast-response control of the ignition timing and combustion duration [1-2].



Fig. 1 RCCI concept. m_1 and m_2 are the mass of low-and high-reactivity fuel.

However, the extension of RCCI combustion under high-load operation conditions is limited by the reactivity of premixed fuel. Its combustion phasing is prone to advance as load increases, which can be counteracted by reducing the amount of high-reactivity fuel.

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This amount tends to decrease to zero as load is high enough. At this point, there is no longer any direct control mechanism over the combustion phasing and combustion process. Moreover, since the port-injected low reactivity fuel is almost premixed, its



Fig. 2 Conceptual illustration of injection strategies of DDFS reproduced from [3]

combustion occurs volumetrically similar to HCCI combustion, resulting in excessively high rates of pressure rise, thus limiting load.

One remedy for extending the load limit of RCCI is to stratify both fuels by injecting gasoline and diesel directly into the cylinder, which allows more flexible controllability over the in-cylinder distribution of two fuels. By using an injection scheme as shown in Fig. 2 [3-5], Wissink and Reitz demonstrated that direct dual fuel stratification (DDFS) is beneficial for distributing heat release rate (HRR) and reducing pressure rise rate (PRR) at high load condition. The advantages of RCCI and partially premixed combustion (PCC) were effectively combined with DDFS by controlling the start of the heat release event with the diesel injection and the peak and duration of the heat release event with near-top dead center (TDC) gasoline injection, DDFS achieved comparable efficiency to that of RCCI, while simultaneously decreasing HRR. However, the effects of the timing of gasoline direct injection on the overall combustion characteristics are not well understood.

In our previous studies [6-13], the ignition characteristics of HCCI, SCCI, and RCCI combustion in constant volume have been investigated. In a real RCCI engine, however, the combustion process including the first-stage ignition is highly affected by both the compression heating before TDC and the expansion cooling after TDC by the piston motion.

The objective of the present study is,

therefore, to investigate the effects of injection timing on the ignition process of the reactivity stratified PRF/air mixture under DDFS conditions using direct numerical simulations (DNSs) with a 117-species reduced primary reference fuel (PRF) oxidation mechanism. The effects of the compression heating and expansion cooling by a piston motion are also accounted for by including mass source term in the governing equations. The simulated motored pressure trace used in the present study is shown in Fig. 3.

The Sandia DNS code, S3D, was used to simulate DDFS combustion process. For all DNSs, the initial pressure and mean temperature of 35 atm and 735 K, respectively. The mean fuel is PRF70 (70% *iso*-octane +



Fig. 3 Experimental and modeled motored-pressure traces as a function of crank angle. Experimental motored-pressure trace taken from experiment by Wissink et al. [3] operating at 1300 RPM under a high-load condition of p_{in} of 1.84 atm.



Fig. 4 Initial equivalence ratio, and PRF fields resulting from (a-b) only n-C₇H₁₆ stratification (top row) and (c-d) both n-C₇H₁₆ and PC₈H₁₈ stratification (bottom row) for DDFS cases 3-5.

30% *n*-heptane by volume). For a typical RCCI combustion concept, *iso*-octane and oxidizer are homogeneously premixed, while *n*-heptane is directly introduced in the cylinder to generate some degrees of mixture stratification. Similar concepts are applied in the present study for Case 2.

DDFS uses an early injection of a portion of gasoline to create a premixed background charge along with a direct injection of diesel to generate some degrees of reactivity and equivalence ratio stratification, followed by a late-direct injection of the remaining gasoline near top dead center (TDC) at the time when the first-stage ignition already completed. To similarly reproduce such multiple injection events and the late iso-octane injection, a pseudo-iso-octane (PC₈H₁₈) model is developed. The effect of injection timing of the late iso-octane injection, t_{ini} is simulated using PC_8H_{18} species. At the beginning of DNSs, PC₈H₁₈ is initialized together with *iso*-octane and n-heptane, and serves as an inert gas. At a specific time, PC₈H₁₈ is converted to iso-octane and become as a fuel to participate in the combustion process.

For DDFS cases (Cases 3-5), both PC₈H₁₈ and *n*-heptane are initialized such that they are inhomogeneously superimposed on a homogeneous iso-octane/air field. Fig. 4a-b and Fig. 4c-d show the initial ϕ and PRF with $n - C_7 H_{16}$, inhomogeneities distributions only and both $n - C_7 H_{16}$ and PC_8H_{18} inhomogeneities, respectively.



Fig. 5 Temporal evolution of mean pressure and $\ensuremath{\mathsf{HRR}}$



Fig. 6 Contours of normalized HRR



Fig. 7 Temporal evolutions of mean mass fraction of fuels, temperature, and HRR.

Figure 5 shows the temporal evolution of mean pressure and HRR for all five cases. As can be readily observed, Case 2 for RCCI shows a higher peak HHR due to a shorter combustion duration compared to DDFS cases. It is attributed to two main reason. First, at high pressure, the ignition delay is deceased exponentially which in turn narrowing the differences in ignition delay time between adjacent fuel/air mixtures. Second, most of charge is well-mixed *iso*-octane/oxidizer and as such, combustion occurs primarily by spontaneous ignition rather than deflagration as revealed in Fig. 6

In contrast, in DDFS combustion (Cases 3-5), the peak HRR and maximum pressure are significantly lower than those of Case 2 (see Fig. 5). Moreover, the overall combustion of DDFS tends to be delayed with advancing the injection timing, t_{inj} . As shown in Fig. 6, Case 3 has more thin flame-like fronts occurring at the early phase of combustion, implying that a mixed combustion mode of deflagration and auto-ignition occurs in the domain. Compared to RCCI, DDFS have a longer combustion duration, which implies that stratification of both fuels is superior to stratification of *n*-heptane only in controlling combustion phasing and alleviating the peak HRR and PRR

Compared to Cases 3-4, the combustion of Case 5, however, proceeds differently with less flame propagation fronts, dominated bv spontaneous ignition. The lower peak HRR compared to RCCI Case 2 is primarily attributed to the rate of supplying iso-octane late injection represented by a process of converting PC₈H₁₈ to iso-C₈H₁₈. As shown in Fig. 7b, the rate of heat release raise coincides with the rate of PC_8H_{18} consumption such that the burn rate during this state is primarily governed by diffusion-limited injection.

In summary, the DDFS combustion concept with stratification in both *iso*-octane and *n*-heptane offers a great potential in extending the upper load limit of DDFS by allowing the flexible capability of manipulating its combustion process.

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