

HCCI조건에서의 희박 PRF/공기 혼합물의 냉염과 열염에 대한 첨가제의 효과에 관한 직접수치모사

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DNSs Study of the Effect of Additives on Cool and Thermal Flame of Lean PRF/Air Mixture under HCCI Conditions

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ABSTRACT

The effects of additives including formaldehyde (CH_2O) and hydrogen peroxide (H_2O_2) for the control of ignition of PRF/air mixture in homogeneous charge compression ignition (HCCI) engines has been investigated by direct numerical simulations (DNSs) with a 118-species pseudo reduced kinetic mechanism. It is found that the overall HCCI combustion of dual additives injection occurs at appropriate time and its mean heat release rate (HRR) is more distributed over time than those of no additive injection.

Key Words : DNS, HCCI, Dual additive, Formaldehyde, Hydrogen peroxide

Homogeneous charge compression-ignition (HCCI) is a combustion process that has some advantages over both spark-ignition (SI) engines and compression ignition (CI) engines. Based on the concept of low temperature combustion in premixed fuel-air mixture and lean burn combustion, HCCI engines have a potential of high thermal efficiency, and low NO_x and particulate matter emissions. HCCI engines, however, have many technical hurdles such as controlling the excessive pressure rise rate (knocking) due to instantaneous ignition of the homogeneous charge [1]. The excessive pressure rise can be alleviated by introducing additive injection. Since an HCCI engine has no combustion-initiating device, the spontaneous auto-ignition is mainly controlled by chemical reactions of fuel and additive.

In many previous DNS studies [2-6], the ignition characteristics of primary reference fuel (PRF)/air mixtures exhibiting two-stage ignition were investigated and as such, the effect of the negative-temperature coefficient (NTC) regime on HCCI combustion was appreciated [7]. The first-stage ignition is

related to low-temperature chemistry (LTC) and the second-stage ignition is associated with the high temperature chemistry (HTC) regime [5]. The first-stage ignition is also regarded as cool flame which has drawn attention due to its profound effects on ignition timing at which the in-cylinder temperature reaches a subsequent thermal flame.

Generally, activation energies of initiation reactions for the additives are lower than those for fuels. As such, small amounts of additives (secondary fuels) can play a significant role in controlling ignition timing. For these reasons, many researchers have studied the effects of additives on IC engine combustion and proposed several methods for enhancing or retarding ignition timing [8-10]. Various additives with different ignition delay characteristics are supplied into the engine cylinder to control the combustion process efficiently. Fuel and oxidizer are first supplied through port fuel injection (PFI) to produce well-premixed charge, followed by one or two direct injections (DI) of additives to generate spatial inhomogeneities in reactivity. By adjusting the amounts of additives and the DI timing of each additive, we can spread out heat release rate (HRR) and alleviate the knocking at the top dead center (TDC), which consequently extends the high-load limit of HCCI engines.

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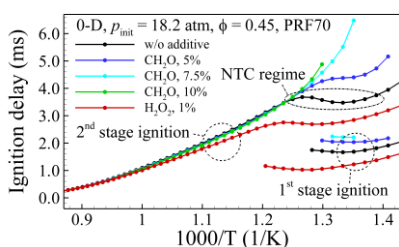


Fig. 1 Effects of CH_2O and H_2O_2 additive on the ignition delay, τ_{ig}^0 , of the PRF70/air mixture with initial pressure of 18.2 atm (-25°CA ATDC)

Figure 1 shows the ignition delay as a function of initial temperature for different additive amounts. The behavior of formaldehyde (CH_2O) changes from a retarder to a promoter within the NTC regime. CH_2O , one of the typical intermediates out of the LTC of hydrocarbon fuels, can be an effective fuel additive for controlling the ignition timing. The addition of CH_2O retards the ignition timing, compared to that without addition. This is because H_2O_2 formation during cool flame is reduced by adding CH_2O . On the contrary, CH_2O is found to slightly advance the overall ignition timing of HCCI combustion at $T = 800$ K or above. However, hydrogen peroxide (H_2O_2) addition results in advanced ignition timing. In general, it is argued that $\text{H}_2\text{O}_2 + \text{M} \rightarrow \text{OH} + \text{OH} + \text{M}$ is the most important reaction in ITC and HTC regime. [5,6,8,10] In other word, H_2O_2 enhances the process from cool flame to thermal flame.

The ignition timing can be controlled by adding promoters or retarders, which, however, may reduce engine efficiency due to inappropriately early or late main ignition timing. To adjust the ignition timing, two different additives, which have opposite ignition delay characteristics, are directly injected in the engine cylinder. Through dual additives injections, relatively gradual ignition process occurs at appropriate ignition timing to prevent knocking problems as well as reducing engine efficiency.

The objective of the present study, therefore, is to provide a better understanding of the effects of the injection of the single and dual additive on PRF/air mixture under HCCI conditions using DNSs by varying three key parameters: (1) temperature fluctuation, (2)

amounts of additives, (3) injection timing of additives under same initial conditions can be examined.

Direct numerical simulations (DNS) were performed to investigate the effect of additives on the HCCI combustion using S3D, which was linked with CHEMKIN and TRANSPORT software libraries. S3D solves the compressible Navier–Stokes, species continuity, and total energy equations. An eighth-order central differencing scheme and a fourth-order explicit Runge–Kutta method were employed for spatial discretization and time integration, respectively. The computational domain is a 2–D square box with each size, L , of 3.2 mm. The number of grids considered is 1280^2 resulting in grid resolution of $2.5 \mu\text{m}$. The boundary conditions are set as periodic in both directions. Initially, the turbulent velocity fluctuations are superimposed on the zero mean velocity field according to the Passot–Pouquet turbulent kinetic energy spectrum function. For all 2–D DNSs, the most energetic length scale, $l_e = 1.737$ mm, is chosen. Turbulence intensity, u' , of 0.5 is deliberately selected to ensure that the turbulence time scale, $\tau_t = l_e/u' = 3.474$ ms $\sim \tau_{ig}$ in a real HCCI engine. The compression heating and pseudo-species models [6] are adopted in present DNSs.

Table 1 Injection timing and amounts of additives (1D)

Type	T'	CH_2O (%)	H_2O_2 (%)	CH_2O (ms)	H_2O_2 (ms)
Single CH_2O	15K	5, 7.5, 10	0	0, 1, 2	–
Single H_2O_2		0	1, 2.5, 5	–	0, 1, 2
Dual additives		20	1, 2.5, 5	0	0~1
Dual additives	30K	10	1	0	0~1

Table 2 Injection timing and amounts of additives (2D)

Type	T'	CH_2O (%)	H_2O_2 (%)	CH_2O (ms)	H_2O_2 (ms)
Single CH_2O	30K	10	0	0	–
Single H_2O_2		0	1	–	0
Dual additives		10	1	0	0.5

In the parametric study, the combined effect of injection timing and amounts of additive on the ignition of a lean PRF/air mixture is investigated (see Table 1, 2). 5~20% volume fraction of CH₂O and 1~5% volume fraction of H₂O₂ are added to the fuel/air mixture, while keeping the equivalence ratio the same as $\phi_0 = 0.45$. To save computational cost, all the simulations start at -25 °CA ATDC, at which the injection of PRF is assumed to be already finished. For all DNSs, mean temperature, pressure and fuel PRF are 760 K, 18.2 atm and PRF 70 at -25 °CA ATDC, respectively. In a recent experimental study [11], the RMS of temperature fluctuation in an HCCI engine was found to be 13.3 K at TDC which is corresponding to 15 K in numerical simulations. For 2D DNSs, initial value of temperature fluctuation, T' of 30 K, is selected to match T' at TDC with experimental results. This is because turbulent mixing reduces the temperature fluctuation in half at TDC. There are many parameters, such as injection timings and amounts of additives to control ignition timing. 0-D and 1-D simulations have also been performed for various amounts and injection timings of additives to make up for 2-D results.

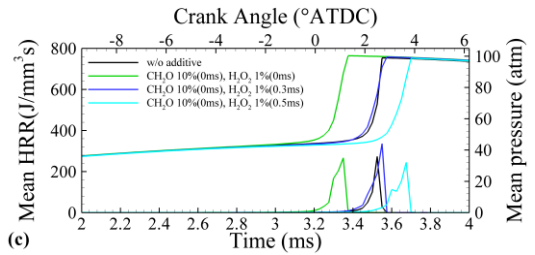
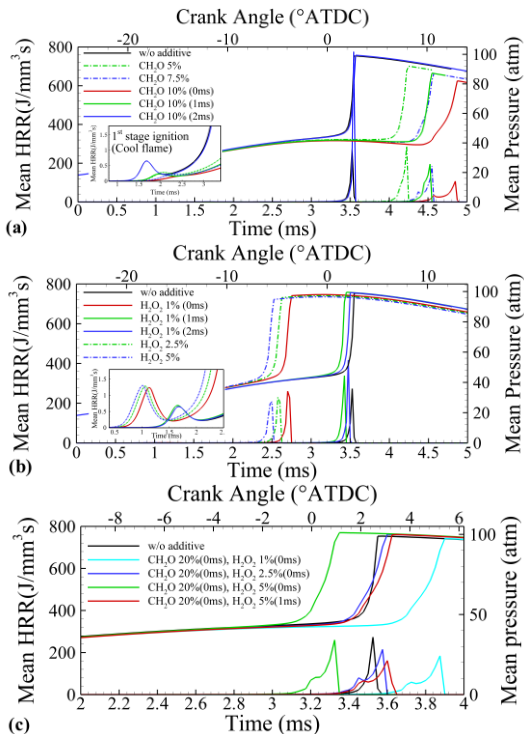


Fig. 2 Temporal evolutions of mean HRR and mean pressure for (a) the injection of single CH₂O ($T' = 15$ K), (b) H₂O₂ ($T' = 15$ K), and (c) the dual additive injections with $T' = 15$ K, (d) $T' = 30$ K.

Figure 2 shows the temporal evolution of the mean pressure, \bar{p} , and HRR, \bar{q} , for single and dual additive injection. First, for the single injection of CH₂O, the ignition timing is monotonically retarded with increasing amount of CH₂O by suppressing generation of cool flame. Consequently, a lot of CH₂O lead to cause misfire. The change of amounts of H₂O₂, however, is not prominent in reducing ignition delay. Second, a later injection (after timing of cool flame generation) of CH₂O and H₂O₂ does not affect ignition timing. In other words, the second-stage ignition timing is subsequently controlled by both CH₂O and H₂O₂ involved in the generation of cool flame. Third, compared to the injection of CH₂O, H₂O₂ addition is effective for changing the ignition delay due to rapid OH radical pool formation. Fourth, for dual additive injections to match with the ignition timing of the no additive type, it is readily observed from Fig. 2c and d that the mean HRR is more spread out over time with increasing T' and amounts of CH₂O. To adjust the appropriate ignition timing, relatively smaller amount of H₂O₂ is directly injected than those of CH₂O for dual additive injection.

Figure 3 shows instantaneous isocontours of cumulative (25%, 50%, 95%) and maximum normalized HRR for different additives injection types. The local HRR, \dot{q} , is normalized by the maximum HRR of 0-D ignition, $\dot{q}_m^0 = 1544, 1474, 1550$ J/mm³ for no additives, H₂O₂ and dual additives injections. In case of single CH₂O injection, \dot{q}_m^0 is substituted by the maximum HRR point of 2-D ignition, $\bar{q}_m = 1312$ J/mm³ because 0-D ignition of CH₂O addition yields misfire for $T_0 = 760$ K as shown in Fig. 1.



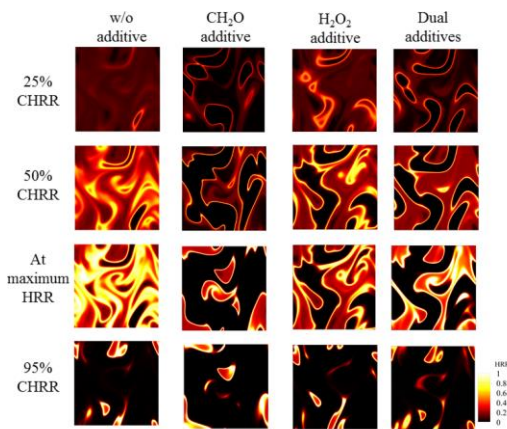


Fig. 3 Isocontours of normalized HRR for no additive, single CH_2O ($T' = 30$ K), single H_2O_2 ($T' = 30$ K) and dual additives ($T' = 30$ K) (from left to right) at times of 25% (first row), 50% (second row) and 95% (last row) cumulative mean HRR and at the maximum HRR (third row).

First, it is readily observed from the first row of Fig. 3 that thin deflagration waves are developed earlier in the additive injection types than in the corresponding no additive type. Second, more deflagrations are generated for additive injection types, i.e. at maximum HRR: ignition kernels evolve into deflagrative waves. On the other hands, the spontaneous auto-ignition dominantly occurs at maximum HRR for no additive injection type. This is because the combustion occurs simultaneously in the domain with high HRR, implying that additive injections induce the deflagration mode of combustion. In general, the deflagration mode of combustion is more apt to spread out the overall HRR than the spontaneous ignition mode. It thus can be employed to alleviate the knocking.

The effects of CH_2O and H_2O_2 addition on PRF70/air HCCI engine combustion were investigated computationally by varying T' , amounts and injection timing of additives. It was found that under same initial mean temperature, pressure and equivalence ratio, T' is significant condition of using CH_2O additive. The amount of CH_2O is limited because CH_2O addition reduces the concentration of OH radical, which plays an important role as the chain carrier. Increment

of the amounts of CH_2O monotonically retards ignition and suppress cool flame generation. It is concluded that CH_2O interrupts formation of cool flame which has considerable influence of generation of thermal flame. Injection timing of H_2O_2 is more important than the amount of H_2O_2 for controlling ignition timing. Dual additive injection can control ignition timing at optimum crank angle degrees with extended range of heat release rate. Deflagration mode is predominant for additive injection types compared to no additive injection. It is elucidated that dual additive injection can be a remedy of engine knocking and improve the quality of combustion.

후 기

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