

A DNS study of CH₂O and H₂O₂ effect on the ignition of lean PRF/air mixtures under HCCI conditions

Jong Hak Kim¹, Gwang Hyeon Yu¹, Minh Bau Luong², Suk Ho Chung², Chun Sang Yoo^{1*}

¹Department of Mechanical Engineering, Ulsan National Institute of Science and Technology
Ulsan 44919, Republic of Korea

² Clean Combustion Research Center, King Abdullah University of Science and Technology
Thuwal, Saudi Arabia

Abstract

The impacts of dual additives including formaldehyde (CH₂O) and hydrogen peroxide (H₂O₂) for the control of ignition of primary reference fuel (PRF)/air mixture in homogeneous charge compression ignition (HCCI) engine conditions have been investigated numerically. It is found that CH₂O addition causes ignition retardation, which may result in a misfire. The chemical effect of CH₂O is to eliminate OH radicals and hence increases the main ignition delay. On the other hand, the addition of H₂O₂ decomposes H₂O₂ into two OH radicals, which promotes the main ignition. It is also found that the overall combustion mode is determined by two different additives with different ignition delay characteristics. For CH₂O and dual additive cases, a mixed combustion mode of both spontaneous ignition and deflagration occurs. However, the spontaneous ignition occurs dominantly in H₂O₂ and no additive cases with short combustion duration. These results suggest that addition of CH₂O provides smooth operation of HCCI engines and besides, dual additive injection can precisely control the ignition timing for HCCI combustion.

1 Introduction

Homogeneous charge compression-ignition (HCCI) engines have been developed as an alternative to conventional gasoline spark-ignition (SI) and diesel compression ignition (CI) engines. High efficiency with low NO_x and particulate emissions in HCCI engines can be usually achieved under lean, dilute, high pressure and low temperature conditions. Despite its advantages over the conventional SI and CI engines, HCCI engines have several problems which remain to be solved such as mitigating excessive pressure rise rate (PRR) and controlling ignition timing under high-load operation conditions [1]. The rapid pressure rise can be alleviated by introducing additive injection. Since an HCCI engine has no combustion-initiating devices, volumetric auto-ignition is mainly controlled by chemical reactions of fuel and additive.

In many previous direct numerical simulation (DNS) studies [2-7], it was found that thermal stratification may effectively control ignition timing and distribute heat release rate (HRR) over time near top dead center (TDC). However, the utilization of thermal stratification is not straightforward and, it still

remains challenging to apply thermal stratification to the development of prototype HCCI engines. Instead, additive injection, which is a secondary fuel, has been proposed as another promising remedy for the problems in HCCI combustion. From extensive experimental and numerical studies by the engine research community, additive was proposed as a strategy to control the ignition timing under HCCI conditions. Many researchers have studied the effects of additives on IC engine combustion and proposed several methods for increasing or decreasing ignition timing [8-12]. For example, formaldehyde (CH₂O) [8-11], and hydrogen peroxide (H₂O₂) [8, 9, 12] are supplied in HCCI engines for a precise control of ignition timing.

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 [2]. The first-stage ignition is noted for its profound effects on the overall ignition timing of HCCI combustion. Both CH₂O and H₂O₂ are produced during the first-stage ignition. CH₂O, one of the typical intermediates out of the first-stage ignition of PRF/air mixture, usually retards the ignition because the formation of H₂O₂ is delayed by CH₂O addition. Below 900 K, CH₂O completely eliminates OH radical. [10] However, H₂O₂ addition advances the overall ignition of PRF/air mixtures. This is because H₂O₂ is one of the most critical species in stimulating the transition from the first-stage to second-stage ignition via a chain branching reaction: H₂O₂ + M → OH + OH + M [8, 9, 12].

The objective of the present study, therefore, is to provide a better understanding of the influences of the single and dual additive injections on PRF/air mixture under HCCI conditions using DNSs by varying amounts and injection timing of additives under same initial conditions can be investigated. The main fuel/air mixture is first supplied via 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 modulating the amounts of additives and the DI timing of each additive, we can spread out HRR over time and alleviate the knocking problem at the TDC, which consequently extends the high-load limit of HCCI engines.

2 Numerical setup and initial conditions

DNSs were performed to investigate the effect of the additive injection strategies on the HCCI combustion using S3D, which is linked with CHEMKIN and TRANSPORT software libraries. Details of the numerical schemes and libraries used in the current

Corresponding author. Fax: +82-52-217-2409
E-mail address: csyoo@unist.ac.kr

study can be found in [7]. 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 attributing to fine grid resolution of 2.5 μm . Periodic boundary conditions were imposed in all directions. Initially, the turbulent velocity fluctuations are superimposed on the zero mean velocity field according to the the Passot-Pouquet turbulent kinetic energy spectrum function. For all 2-D DNSs, the most energetic length scale, $l_e = 1.737$ mm, is selected. 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 engine. The compression heating and pseudo-species models [7] are used in present DNSs.

In the present study, the effects of injection timing and amounts of additives on the ignition of a lean PRF/air mixture are investigated (see Table 1 and 2). 5 ~ 20% volume fraction of CH_2O and 1 ~ 5% volume fraction of H_2O_2 are added to the fuel/air mixture, while keeping the equivalence ratio the same as $\phi_0 = 0.45$. For all DNSs, mean temperature, pressure and fuel PRF are 760 K, 18.2 atm and PRF 70 at -25 °CA ATDC, respectively. To save computational cost, all the simulations start at -25 °CA ATDC, when the injection of PRF is assumed to be already finished. In a recent experimental research [13], 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 2-D DNSs, initial value of temperature fluctuation, T' of 30 K, is selected to match T' at TDC with experimental results, since 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. 1-D simulations have been performed for saving computational time to make up for 2-D results.

3 Results

3.1 Overall combustion characteristics

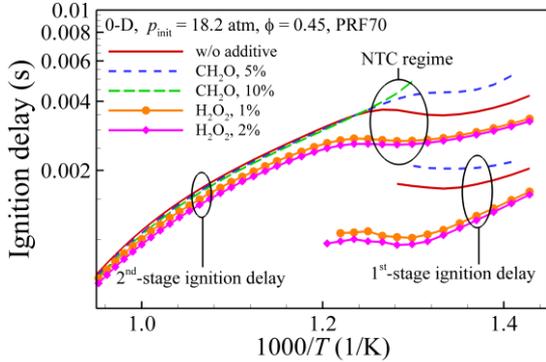


Figure 1: The ignition delay, τ_{ig}^0 , of the PRF/air mixture with CH_2O and H_2O_2 additions

The 0-D ignition delays can be determined by injection of two different additives, which have opposite ignition delay characteristics. Figure 1 shows the ignition delay as a function of initial temperature for different additive amounts. The behavior of CH_2O changes from a retarder to a promoter within the NTC regime. The addition of CH_2O retards the ignition timing, compared to that without addition. 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 advancing 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 the second-stage ignition since H_2O_2 stimulates the process from cool flame to thermal flame.

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 ^a | 5, 7.5, 10 | 0 | 0, 2 | - |
| Single H_2O_2 | | 0 | 1, 2.5, 5 | - | 0, 2 |

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 ^a | 10 | 0 | 0 | - |
| Single H_2O_2 | | 0 | 1 | - | 0 |
| Dual additives | | 20 | 3 | 0 | 0.5 |

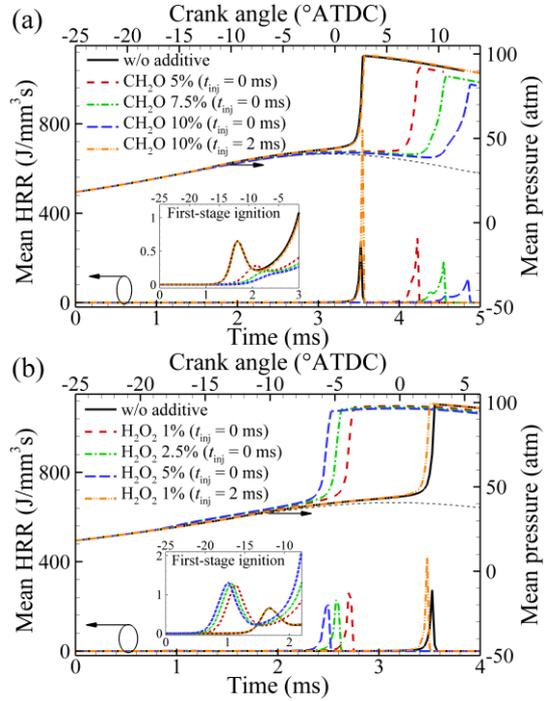


Figure 2: Temporal evolutions of mean HRR, \bar{q} , and mean pressure, \bar{p} , for (a) the injection of single CH_2O , and (b) H_2O_2 with $T' = 15$ K (1-D)

To arrange the value of key parameters such as the amounts and injection timings of additives 1-D cases are simulated for single additive injection. 1-D simulations are performed to compare with the 2-D results under the corresponding compression heating conditions. Figure 2 shows the several distinct behaviors of the first- and second-stage ignition depending on the injection types of the additives. First, for the single injection of CH_2O (see Fig. 2a), it is readily observed from the figure that CH_2O 10% case exhibits much lower peak HRR and longer combustion duration than CH_2O 5% case. The ignition timing is monotonically retarded with increasing amount of CH_2O by suppressing generation of cool flame. The variation of τ_{ig} between pure fuel case and CH_2O injection cases for 5%, 7.5% and 10% are 0.71, 1.03 and 1.33 ms, respectively. Although combustion phasing retarder allows higher loads because of

slowing the PRR, the excessive amount of retarder is prohibited by poor cycle-to-cycle stability and eventually causes a misfire. For the single injection of H_2O_2 (see Fig. 2b), the ignition timing is non-monotonically increased with increasing amount of H_2O_2 . The variation of τ_{ig} between the pure fuel case and H_2O_2 injection cases for 1%, 2.5% and 5% are 0.82, 0.94 and 1.02 ms, respectively. The change of amounts of H_2O_2 is not prominent in reducing ignition delay. Regardless of the amounts of H_2O_2 , the HRR of first-stage ignition becomes twice for H_2O_2 injection cases. The injection of H_2O_2 improves the reactions for the generation of cool flame.

Second, a later injection (after timing of cool flame generation) of CH_2O and H_2O_2 does not affect second-stage ignition timing. Especially, the first-stage ignition timings are almost the same for with and without additives. In other words, the main ignition timing is controlled by both CH_2O and H_2O_2 highly involved in first-stage ignition reactions. The influence of additives is intensified with earlier injection timing. To maximize their effect on HCCI combustion, the additives may be injected as soon as possible or by PFI.

Third, it is found that H_2O_2 addition is effective in changing the ignition delay, compared to the CH_2O addition for a fixed quantity of additives. For example, CH_2O 5% and H_2O_2 5% addition change the ignition delay 0.7 ms and 1.02 ms, respectively. This is because CH_2O eliminates one OH radical at low-temperature chemistry (LTC) regime [6], but H_2O_2 rapidly decompose two OH radicals.

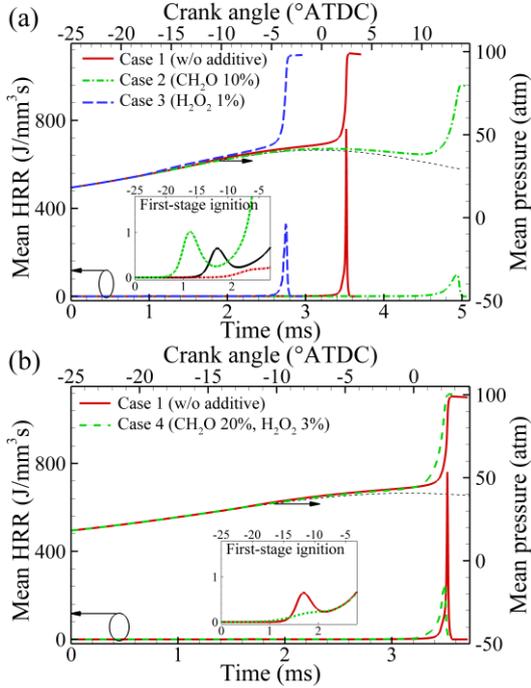


Figure 3: Temporal evolutions of mean HRR, \bar{q} , and mean pressure, \bar{p} , for (a) the injection of single CH_2O , H_2O_2 , and (b) the dual additive injections with $T' = 30 \text{ K}$ (2-D).

Figure 3 shows the temporal evolution of the mean pressure, \bar{p} , and HRR, \bar{q} , for single and dual additive injection. First, for the effects of single injection of CH_2O , and H_2O_2 are similar with 1-D simulation results. It means the effects of the random spectrum of turbulence and temperature on overall combustion process are marginal.

Second, for dual additive injections to match with the ignition

timing of the no additive type, it is readily observed from Fig. 3b that the mean HRR is more spread out over time for Case 4.

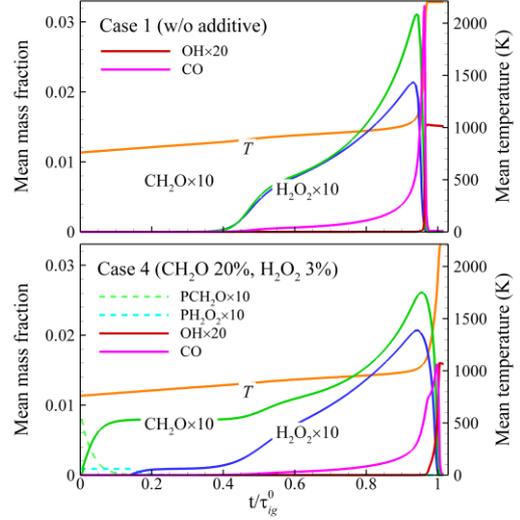


Figure 4: Temporal evolutions of the mean mass fraction of the important minor species, and temperature for Cases 1 (top) and 4 (bottom)

To verify the effect of additive on the overall combustion process of Cases 1 and 4, the temporal evolutions of the mean mass fractions of important minor species are shown in Fig.4 together with those of the mean temperature. It is readily observed from the figure that for Case 1, the mean mass fractions of CH_2O and H_2O_2 increase at first-stage ignition. For Case 4, however, those of CH_2O and H_2O_2 increases right after the conversions of PCH $_2\text{O}$ to CH_2O and PH $_2\text{O}_2$ to H_2O_2 , and then also increases at first-stage ignition. Moreover, the peak mass fraction of CO for Case 4 is less than that for Case 1. These results demonstrate that for Case 4, additions of CH_2O and H_2O_2 lead the complete combustion and maintain the same main ignition timing with Case 1.

3.2 Combustion mode analysis

To further investigate the characteristics of instantaneous HCCI combustion mode, the isocontours of normalized HRR for Cases 1 - 4 are shown in Fig.5. As shown in the figure, it is readily observed from the first row that strong heat release occurs in several thin deflagration waves, which develop earlier in cases with CH_2O and dual additive injections than in cases without additives. This result implies that CH_2O injection induces the mixed combustion mode. On the other hands, the combustion of no additive and H_2O_2 injection cases seem to occur over a broad area by spontaneous auto-ignition. This is because the combustion occurs simultaneously in the domain with high HRR. 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.

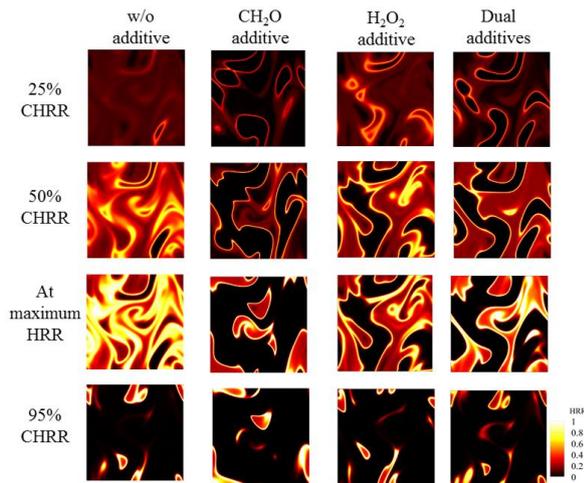


Figure 5: Isocontours of normalized HRR for no additive, single CH₂O, H₂O₂ and dual additives (from left to right) at times of 25% (first row), 50% (second row) and 95% (last row) cumulative mean HRR and at the maximum HRR (third row)

4 Conclusions

The effects of CH₂O and H₂O₂ addition on PRF70/air HCCI engine combustion were investigated numerically by varying the amounts and injection timing of additives. It was found that under the same initial mean temperature, pressure and equivalence ratio, the role of CH₂O in ignition changes from a retarder to a promoter as the temperature increment. The amount of CH₂O is limited because CH₂O addition reduces the concentration of OH radical, which plays an important role as the chain reaction carrier. It is concluded that CH₂O interrupts formation of cool flame which has a considerable influence on the start of the main ignition. On the other hands, the main ignition timing is only promoted with increasing H₂O₂ amount. Dual additive injection can control ignition timing at optimal crank angle degrees with distributed range of HRR over time. Deflagration mode is predominant for CH₂O and dual injection types compared to no additive injection. These results demonstrate that dual additive injection can allow a precise control of combustion phasing and peak HRR by adjusting the amount and injection timing of CH₂O and H₂O₂. Moreover, derived smooth operation of HCCI engines can be a remedy of engine knocking and improve the quality of combustion.

5 Acknowledgment

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