Effect of Hydrogen Blending on the Combustion Performance of a Gasoline Direct Injection Engine

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ABSTRACT: To explore the effect of hydrogen blending on the combustion of a gasoline direct injection engine, a three-dimensional model of the engine is built. The effects of some hydrogen volume fractions (HVFs) and ignition timings (ITs) on the engine performance parameters are studied. Furthermore, the microstructure and mechanism of combustion are analyzed. The simulation results reveal that when the gasoline engine is blended with hydrogen, the active hydroxyl radical concentration increases, and the combustion process is accelerated. When the IT is fixed, with the HVF rising, the peak heat release rate and cylinder pressure will increase. The ignition delay, combustion duration, and crank angle when cumulative heat release reaches 50% decrease. Additionally, the autoignition is shifted to an earlier time as the IT advances. Under the studied conditions with the increase in the HVF, the knock resistance is enhanced because hydrogen has a high knock resistance and octane number.

1. INTRODUCTION

Since the last century, fossil fuels have become the major source of energy worldwide. Owing to the rapid development of the world economy, the demand for energy is increasing. This has accelerated the depletion of fossil fuels. In addition, environmental pollution and health problems caused by the burning of fossil fuels are becoming increasingly serious. It is estimated that the transportation sector consumes nearly two-thirds of the oil consumed worldwide. With the aggravation of energy crises and environmental problems, researchers have started to focus on blended fuels or alternative fuels, such as biogas, biodiesel, methanol, ethanol, dimethyl ether, and reforming gas, to improve the engine thermal efficiency or reduce emissions.

Hydrogen, as a renewable and clean resource, has drawn extensive attention. Compared with traditional fuels, such as gasoline and diesel, hydrogen exhibits the features of a higher laminar flame velocity, shorter quenching distance, and higher diffusion coefficient. However, hydrogen as an engine fuel also faces problems such as safety, preignition, backfire, and power reduction. It can effectively improve fuel vaporization and mixture, speed up combustion, and decrease cold wall quenching and cyclic variations when hydrogen is introduced into a gasoline engine. Furthermore, mixing hydrogen can bring the engine closer to the ideal constant volume combustion, which can increase the thermal efficiency.

Many researchers explored the influence of the hydrogen inlet port injection on the combustion of gasoline engines. Ceviz et al. reported that the fuel consumption rate decreased by approximately 12% when the hydrogen volume ratio corresponded to 5.28%. Furthermore, the indicated thermal efficiency (ITE) improved by approximately 18% and hydrocarbon (HC) emissions decreased by 13%. However, NO emissions increased as the in-cylinder gas temperature increased. Baghdadi et al. reported a decrease in CO emissions by 49% using a blend of 4% hydrogen and 30% ethanol. Additionally, NOX emissions were reduced by 39%, and the thermal efficiency and output power
improved. D’Andrea et al.21 studied the influence of hydrogen on engine combustion under different operating conditions. The results indicated a decrease in the combustion duration and cyclic variation with a rise in hydrogen addition. Jingding et al.22 investigated the emission formation mechanism of a hydrogen–gasoline engine and observed that HC and CO emissions were significantly reduced by supplying hydrogen during the lean burn. Karagöz et al.23 observed the performance and emissions of gasoline engines by varying the hydrogen energy fractions. The results revealed an improvement in the cyclic variation, indicated mean effective pressure, ITE, indicated specific fuel consumption, and peak temperature with an increase in hydrogen blending fractions. However, hydrogen blending led to an increase in NO\textsubscript{X} emissions. Elsimary et al.24 observed the influence of different volume ratios of hydrogen blending on an engine. The results demonstrated that hydrogen blending accelerated the combustion rate of the mixture and increased the cylinder pressure. Furthermore, engine performance tests revealed an improvement in the ITE with the addition of hydrogen. Karagöz et al.25 introduced the H\textsubscript{2}/O\textsubscript{2} mixture into the intake port and revealed an improvement in the braking power and ITE.

Although hydrogen blending can make the combustion better and the ITE higher, it can also significantly increase NO\textsubscript{X} emissions. To resolve this problem, some researchers observed the influence of exhaust gas recirculation (EGR) on hydrogen–gasoline engines. Saravanan et al.26,27 examined the effects of hydrogen injection at different flow rates on hydrogen–gasoline engine performance under different EGR ratios. They determined that the ITE increases by 6% and the NO\textsubscript{X} concentration is reduced by EGR when hydrogen is added at the rate of 20 L/min. When 25% EGR was used, the minimum concentration of NO\textsubscript{X} was 464 ppm, HC emissions decreased by 58%, and soot emissions were reduced by 52%. Kim et al.28 studied the effects of hydrogen on the ITE and emissions of a turbo gasoline direct injection (GDI) engine with EGR. The results revealed that hydrogen mixing can increase the operable EGR rate, increase the combustion rate, and reduce the cyclic variation. Specifically, under high EGR rate conditions, the pressure differences between cylinders with different braking average effective pressure values decreased as the hydrogen blending ratio increased. The improved combustion and higher EGR rate, which can reduce heat loss, led to an improvement in the ITE. Yu et al.29 studied the influence of hydrogen blending on gasoline engines under some excess air coefficient conditions. The results revealed an initial increase followed by a subsequent decrease in the thermal efficiency as the excess air coefficient was increased. Hydrogen blending can stabilize ignition, accelerate combustion, and enhance braking thermal efficiency. Furthermore, owing to more complete fuel combustion, CO and HC emissions decreased. However, additional NO\textsubscript{X} was produced because of the higher combustion temperature. At an EGR rate of 18% and an excess air coefficient of 1.0, 1.2, and 1.4, NO\textsubscript{X} emissions declined significantly, with maximum reductions of 82.7, 77.8, and 60%, respectively.

To avoid a decrease in the volumetric efficiency of hydrogen port injection, some researchers investigated the combination of gasoline port injection and hydrogen direct injection (HDI). Yu et al.30 studied the influence of HDI on a gasoline engine and optimized the main parameters in the experiment such as an excess air coefficient and load. The results revealed that hydrogen blending enhances the braking thermal efficiency and improves the lean-burn performance. The combustion duration was reduced by approximately 20% with the addition of 10% hydrogen to gasoline. Furthermore, they observed the effect of HDI on the particulate matter. They observed a decrease in the number of nucleating particles, and more aggregated particles were observed when the equivalence ratio corresponded to 1.1. Under the extra-lean condition, the change in the hydrogen fraction slightly affected the number of particles, thereby indicating that the influence of the carbon–oxygen ratio was higher when compared to that of the equivalence ratio on the formation of particles.31 Du et al.32 observed the influence of EGR on the combustion and emissions of a port injection gasoline engine with HDI. The peak pressure of the cylinder was enhanced by 9.8%, and the engine torque was increased by 11% due to hydrogen blending. In addition, NO\textsubscript{X} emissions were reduced by 45.2% due to EGR when compared to those of the original engine.

Based on the abovementioned analysis, hydrogen blending can improve the combustion and emission performance of engines. However, research on the flame development and the hydrogen–gasoline combustion mechanism is limited. In addition, so far, the hydrogen–gasoline engine knock phenomenon has rarely been reported. In this study, we aim to examine the influence of hydrogen volume fraction (HVF) and ignition timings (ITs) on the combustion of a hydrogen–gasoline engine via a computational fluid dynamics method. Furthermore, the combustion and knock were analyzed in terms of reaction mechanisms. Aiming to find features of the knock of hydrogen–gasoline and its influence on the internal combustion engine, it is expected that our findings can serve as a reference for related research.
2. NUMERICAL MODEL AND VALIDATION

In this study, a three-dimensional (3D) model of a 1.5T GDI engine was established in SolidWorks. Then, the model was transformed into an STL format file as the input file in simulation software CONVERGE. The engine model and parameters are presented in Figure 1 and Table 1, respectively. Also, in order to get more detailed information about mixture autoignition, eight monitor points (P1–P8) were uniformly set in the combustion chamber.

Table 1. Parameters of the Engine

| parameter                   | value   |
|-----------------------------|---------|
| bore diameter/mm            | 75      |
| stroke/mm                   | 84.6    |
| compression ratio           | 9.8     |
| intake valve open (° CA BTDC)| 30      |
| exhaust valve open (° CA ATDC)| 149     |

2.1. Numerical Model. The flow field in the engine cylinder is highly complex because of fluid flow, chemical reactions, heat, and mass transfer. Hence, appropriate models must be selected to predict fluid flow and chemical reactions in the cylinder with high accuracy. Several studies indicated that the SAGE model\(^{34,35}\) is appropriate for the simulation of gasoline engine combustion with high accuracy, and thus it was selected as the combustion model in this study. Other models, such as the turbulence model and the spray model, should be selected based on the scenarios to be examined. The models utilized in this paper are listed in Table 2.

Table 2. List of Sub Models

| model                        | sub model               |
|------------------------------|-------------------------|
| turbulence model             | K–ε double equation model|
| fuel fracture model          | RT-KH fracture model    |
| collision mode               | NTC collision model     |
| spray-wall interaction model | wall film model          |
| combustion model             | SAGE model              |

2.2. Initial Conditions. Accurate initial and boundary conditions have an important effect on the simulation accuracy. The initial conditions and boundary conditions of this study were set according to the experiments and GT-power simulation results. Some initial and boundary conditions are listed in Table 3. During the entire simulation process, the total energy of gasoline and hydrogen remained constant under all the conditions. Also, the hydrogen was introduced in the intake manifold behind the turbocharger. Specifically, the HVF and mass of gasoline injected per cycle were, respectively, calculated in eqs 1 and 2.

\[
\alpha_{H_2} = \frac{V_{H_2}}{V_{H_2} + V_{air}} \quad (1)
\]

\[
m_{gasoline} = (V_{air} \rho_{air} - V_{H_2} \rho_{H_2} \lambda_{F_{st,H_2},H_2}) / \lambda \rho_{gasoline} \quad (2)
\]

In eqs 1 and 2, \(V_{H_2}\) and \(V_{air}\) denote the volumes (L) of hydrogen and air, respectively; and \(\rho_{H_2}\) and \(\rho_{air}\) denote the densities of hydrogen and air, respectively (g/L); \(F_{st,H_2}\) and \(\lambda_{F_{st,H_2},H_2}\) denote the air-fuel stoichiometries of hydrogen and gasoline, respectively; and \(\lambda\) denotes the excess air coefficient.

2.3. Knock Intensity Evaluation. Minor knocks can promote combustion and improve the ITE of the engine, while severe knocks can worsen combustion. In this paper, the knock intensity (KI) is defined as the average of the maximum amplitude of pressure oscillations (MAPO) of the monitors\(^{36}\) as follows

\[
KI = \frac{1}{N} \sum_{i=1}^{N} \max (\hat{P}^0_{i,\theta_0}) \quad (3)
\]

where \(\hat{P}\) is the band-pass filtered pressure of the monitor \(\theta_0\), and \(\theta_0\) denotes the start crank angle of the filter window, and \(\omega\) denotes the width of the filter window. A larger KI means more severe knock combustion.

2.4. Model Validation. CONVERGE includes an adaptive mesh refinement function that can automatically encrypt regions based on the requirements of the calculation process and regions. Hence, it ensures accuracy and speed in calculations. To enhance the calculation efficiency and satisfy accuracy requirements, a 4 mm basic grid was used, and some regions, such as those near the cylinder liner, piston, and intake and exhaust valves, were encrypted to different degrees.

To accurately simulate the operating process of the engine, the numerical simulation results were validated via experimental results when the engine, respectively, operated at 3000 rpm-272.2 N m and 2500 rpm-266.9 N m. A comparison between the experimental and simulation results for the in-cylinder pressure is shown in Figure 2. As shown in the figure, the simulation value is in good agreement with the experimental value. The maximum values of the experimental cylinder pressure were, respectively, 7.88 and 7.19 MPa when the engine operates at 3000 rpm-272.2 N m and 2500 rpm-266.9 N m. The errors were about 0.1%. The errors are calculated by eq 4. Based on the model, a simulation of the combustion of different hydrogen–gasoline blending was performed. The operation conditions of the engine used in the paper are listed in Table 4. The results of the simulation are discussed in the following sections.
Table 4. Operation Conditions of the Engine

| Parameter                              | Value          |
|----------------------------------------|----------------|
| Speed (rpm)                            | 2500           |
| Gasoline injection time (° CA ATDC)    | −261           |
| Gasoline injection pressure (MPa)      | 15.0           |
| Hydrogen volume fraction (%)           | 0.0, 2.0, 4.0, 6.0, 8.0, 10.0 |
| Ignition timing (° CA ATDC)            | −11.0, −7.0, −5.0, −3.0, −1.0, 1.0, 2.0 |

error = \left( \frac{E_{\text{value}} - S_{\text{value}}}{E_{\text{value}}} \right) \times 100%  \tag{4}

where \( E_{\text{value}} \) denotes the maximum pressure in the experiment and \( S_{\text{value}} \) denotes the maximum pressure in the simulation.

3. RESULTS AND DISCUSSION

3.1. Influence of the HV on Combustion. Figure 3 shows the maximum cylinder pressure (\( P_{\text{max}} \)), heat release rate (\( \text{HRR}_{\text{max}} \)), and corresponding crank angle of different HVFs with an intake pressure of about 2.0 bar. Also, the excess air coefficient of the mixture is 1.0 in all the studied conditions. As the figure shows, the \( P_{\text{max}} \) and \( \text{HRR}_{\text{max}} \) increase as the HVF increases, and their phases gradually advance. This is due to hydrogen blending, which increases the combustion rate and makes the heat release more concentrated. However, as the IT is advanced, the difference in \( P_{\text{max}} \) among different HVFs gradually decreases. Under the same HVF, the \( \text{HRR}_{\text{max}} \) basically increases with the advance of IT. Furthermore, \( P_{\text{max}} \) also increases in the same trend. It can be seen from Figure 3c that under most working conditions, the curves of the HRR have only one peak. However, under the low HVFs and earlier IT working conditions, the curves of the HRR have two peaks, as shown in Figure 3e, the HRR with 2.0% HVF at different ITs. It is thought to be the result of autoignition combustion of the end-gas and knock.

3.2. Effect of HV and IT on the Combustion Phase. The influences of the HV and IT on the ignition delay period and combustion duration are shown in Figure 4a,b, where the ignition delay period refers to the crankshaft angle from the ignition start point to 10% fuel combustion, and the combustion duration refers to the crankshaft angle from 10% fuel combustion to 90% fuel combustion. As shown in Figure 4a, in the case of the fixed IT, when the HVF changes from 0.0 to 10.0%, the ignition delay gradually decreases, especially when IT is late. The phenomenon that the ignition delay decreases with the increase of the HVF can be explained from the perspective of
chemical reaction kinetics. Macromolecular HCs in gasoline fuel are not easily ignited and burned in a low-temperature stage. The following correspond to several reaction equations involved in the gasoline oxidation process

\[
\begin{align*}
RH + O_2 & \rightarrow R^* + HO_2 \\
R^* + O_2 & \rightarrow RO_2 \\
RO_2 + RH & \rightarrow R^* + ROOH \\
RO_2 & \rightarrow R^*CH_3O \rightarrow R^* + CH_2O \\
ROOH & \rightarrow RO + OH \\
RCHO/CH2O + RO_2 & \rightarrow RC^*O/CHO + ROOH \\
R^* + O_2 & \rightarrow olefin + HO_2 \\
RH + HO_2 & \rightarrow R^* + HOOH
\end{align*}
\]

In the abovementioned reactions, RH denotes alkanes, R, R*, and R'' denote the alkyl radical, RO2 denotes the alkylperoxy radical, and M denotes the third body.

However, when the gasoline engine mixed with hydrogen, more free radicals H produced in the low-temperature reaction zone increased (as shown in chemical reaction eq 13), and the chain reaction (such as eqs 14−16) promoted the formation of free radicals OH by consuming free radicals H. This speeds up the oxidation reaction of the hydrogen–gasoline mixture, thus reducing the ignition delay.

\[
\begin{align*}
H_2 + M & \rightarrow H + H + M \\
H + O_2 + M & \rightarrow HO_2 + M \\
HO_2 + CH_3 & \rightarrow OH + CH_3O \\
H + H_2O & \rightarrow OH + H_2
\end{align*}
\]

Moreover, under the same HVF, the ignition delay first decreases and then increases with the advance of IT. This is because the ignition delay is also limited by temperature and cylinder pressure. Therefore, when the IT is too early, the ignition delay increases slightly, owing to the relatively lower temperature and pressure in the cylinder.

As for the combustion duration, it is shortened at a fixed IT with the increase of HVFs and also shortened at a fixed HVF with the advancement of ITs. However, when the HVF is about 8.0%, the combustion duration increases when IT is early. This is because the knock resistance of the mixture improves with the increase of hydrogen. Moreover, with the advance of IT, part of the fuel will be consumed in the relatively low temperature and pressure stage, thus reducing the autoignition of end-gas and prolonging the combustion duration.

The combustion event must be properly phased relative to the top-center piston position to obtain the maximum power or torque. The CA50 is also an important index for evaluating the engine combustion phase. The CA50 values under different ITs and HVFs are shown in Figure 5. At a given excess air coefficient (1.0) and fixed IT, CA50 is progressively advanced with the rise of HVFs. Also, for a fixed HVF, the CA50 is also advanced with the rise of IT, which indicates that the increase in the HVF and advanced IT causes the duration of the flame development and the propagation process to shorten. For an optimal CA50 phase, the IT of the hydrogen–gasoline engine must be controlled to obtain the maximum power or torque at different HVFs.

3.3. Effect of the HVF on Flame Propagation. To examine the combustion process of a gasoline engine using a hydrogen–gasoline blend, a 3D field analysis of the flame propagation is conducted. In this study, the flame front was characterized via a temperature isosurface with \( T = 1700 \) K. In addition, the IT is 1° CA after top dead center (ATDC) for different HVFs. Figure 6 shows the flame development and the distribution in the cylinder at different crank angles under different HVFs. In the early stages of ignition, a flame center rapidly forms near the spark plug, and the flame center spreads gradually. Given the effect of the flow field and the distribution of the unburned mixture, the shape of the flame front is irregular at different times. It should be noted that the range of flame propagation gradually increases when the HVF increases at the same crank angle, which implies that an increase in the HVF speeds up the flame propagation. The results of the flame propagation simulation revealed that the hydrogen additive can
accelerate combustion and the heat release, which agrees well with the results shown in Figures 3 and 4.

3.4. Influence of the HVF and IT on the ITE and Knock. Figure 7 shows the ITE, heat loss, cylinder pressure, and knock for different HVFs and ITs. As shown in Figure 7a, the ITE difference is more evident with IT delay, thereby indicating that the influence of hydrogen on combustion acceleration is more obvious for later ITs. As the IT continues to advance, the maximum ITE will be improved a little, and the KI will also increase, as shown in Figure 7d. Figure 7a shows that when it is at the calibrated ignition advance time of a gasoline engine, that is, 2° CA ATDC, with the increase of the HVF from 0.0 to 10.0%, ITE increases from 35.1 to 40.1%. It can also be seen from the figure that a reasonable HVF will improve the maximum ITE
obviously and increase the KI slightly when IT is late. When the ignition angle is earlier, the higher HVF makes the ITE decrease due to the increasing heat loss and compression negative work as shown in Figure 7b,c.

As shown in Figure 7d, when the HVF is less than 4.0% and the IT is earlier than $-7^\circ$ CA ATDC, the knock is more serious, and the KI is greater than 1.0 MPa, which is considered as a serious knock. Especially when the HVF is 2.0% and the IT is $-11.0^\circ$ CA ATDC, the KI is greater than 3.0 MPa. When IT varies from $-7$ to $-11^\circ$ CA ATDC, the KI decreases obviously with the further increase of the HVF, especially the HVF of 8.0%. The abovementioned phenomenon may be explained by the fact that under a low HVF condition, the proportion of gasoline is still high, but due to hydrogen blending, the combustion temperature in the cylinder is higher, which makes the autoignition of the end-gas more serious. With the further increase of the HVF, the anti-knocking performance of the hydrogen–gasoline mixture is improved due to the larger octane number of hydrogen, so the KI decreases.

To further understand the effect of the IT on the combustion knock of hydrogen blending, it is necessary to analyze intermediate products and some phenomena of autoignition during the combustion process in detail. The CH$_2$O, OH, flame propagation, and temperature fields in the cylinder are shown in Figure 8. According to chemical reaction, in the low-temperature oxidation process of alkanes, as the temperature increases, the branched chain reaction of peroxyalkyl (RO$_2$) continues to occur to form formaldehyde (CH$_2$O), which is a typical low-temperature product. Additionally, OH is a high-temperature chemical reaction product and can be used as a mark of ignition. With the formation of OH radicals, CH$_2$O is consumed rapidly in this area, thereby indicating the occurrence of autoignition. The simulation results reveal that the occurrence of autoignition is consistent with CH$_2$O consumption and OH generation at ITs of $-7$ and $-11^\circ$ CA ATDC with 2.0% HVF as shown in Figure 8, respectively. Also, the crank angles of the knock onset at different ITs with 2.0% HVF are shown in Figure 9. As shown in Figure 9, the crank angle of the autoignition onset advances with IT advances. When the IT advances from $-3$ to $-11^\circ$ CA ATDC, the occurrence time of autoignition advances from 26.73 to 11.68° CA ATDC. The occurrence time of autoignition is closer to the TDC, thus the cylinder pressure fluctuation due to the autoignition is more obvious, and the KI increases as the IT increases as shown in Figure 7d. However, the IT has little effect on the autoignition position because IT cannot change the distribution of the mixture, obviously, but IT advances with IT advances.

![Figure 8](image.png)

*Figure 8. Evolution of the temperature isosurface of 1700 K, CH$_2$O, OH, and temperature distributions in the cylinder under different ITs (slice position of temperature, OH, CH$_2$O, and flame propagation is $Z = -0.0241$ m).*

![Figure 9](image.png)

*Figure 9. Crank angle of the knock onset at different ITs with HVF of 2.0%.*
will affect the time it takes for the autoignition position to reach the autoignition temperature and pressure.

4. CONCLUSIONS

In the paper, a 3D engine model was built, and a combustion simulation was conducted to examine the effect of hydrogen blending on GDI engine combustion. The main conclusions are as follows:

(1) An increase in the HVF leads to an increase in the peak cylinder pressure and peak HRR. The crank angle of the peak value is closer to the TDC. When IT advances, peak pressure and HRR increase continuously, although the difference between hydrogen—gasoline and gasoline decreases. At lower HVFs, when IT advances, the knock increases, and the maximum KI can reach more than 3.0 MPa.

(2) When the IT is late, an increase in the HVF from 0 to 10.0% leads to an increase from 35.1 to 40.1% of ITE at IT is 2° CA ATDC. When the IT is too early, the greater HVF makes the ITE lower. At a fixed HVF, as the IT advances, the ITE first increases and then decreases.

(3) The simulation results reveal that when the gasoline engine is blended with hydrogen, the active OH radical concentration increases, and the combustion process is accelerated. In the case of fixed IT, the ignition delay decreases as the HVF increases from 0.0 to 10.0%. With the advance of the IT, the ignition delay gradually decreases, and the combustion duration also exhibits the same trend.

(4) The simulations of the CH$_2$O, OH, flame propagation, and cylinder temperature fields reveal that the occurrence of autoignition is consistent with CH$_2$O consumption and OH generation at different ITs, and the crank angle of the autoignition onset also advances with the IT advancing.

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Notes
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NOMENCLATURE

GDI gasoline direct injection
HDI hydrogen direct injection
ATDC after top dead center
HVF hydrogen volume fraction
IT ignition timing
HRR heat release rate
ITE indicated thermal efficiency
CA50 crank angle when cumulative heat release reaches 50%
IMEP indicated mean effective pressure
$P_{\text{max}}$ maximum cylinder pressure

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