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Effects of Flame Propagation Velocity and Turbulence Intensity on End-Gas Auto-Ignition in a Spark Ignition Gasoline Engine

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Abstract: Knocking is a destructive and abnormal combustion phenomenon that hinders modern spark ignition (SI) engine technologies. However, the in-depth mechanism of a single-factor influence on knocking has not been well studied. Thus, the major aim of the present study is to study the effects of flame propagation velocity and turbulence intensity on end-gas auto-ignition through a large eddy simulation (LES) and a decoupling methodology in a downsized gasoline engine. The mechanisms of end-gas auto-ignition as well as strong pressure oscillation are qualitatively analyzed. It is observed that both flame propagation velocity and turbulence have a non-monotonic effect on knocking intensity. The competitive relationship between flame propagation velocity and ignition delay of the end gas is the primary reason responding to this phenomenon. A higher flame speed leads to an increase in the heat release rate in the cylinder, and consequently, quicker increases in the temperature and pressure of the unburned end-gas mixture are obtained, leading to end-gas auto-ignition. Further, the coupling of a pressure wave and an auto-ignition flame front results in super-knocking with a maximum peak of pressure of 31 MPa. Although the turbulence indirectly influences the end-gas auto-ignition by affecting the flame propagation velocity, it can accelerate the dissipation of radicals and heat in the end gas, which significantly influences knocking intensity. Moreover, it is found that the effect of turbulence is more pronounced than that of flame propagation velocity in inhibiting knocking. It can be concluded that the intensity of the pressure oscillation depends on the unburned mixture mass as well as the local thermodynamic state induced by flame propagation and turbulence, with mutual interactions. The present work is expected to provide valuable perspective for inhibiting super-knocking of an SI gasoline engine.

Keywords: knocking mechanism; flame propagation velocity; turbulence; auto-ignition; pressure oscillation

1. Introduction

The increasing severity of the current energy crisis and environmental pollution are leading to technical downsizing and turbocharging in spark ignition (SI) engines due to their superior economy and power performance [1]. Theoretically, the engine performance, such as the torque and fuel consumption rate, is positively related to the fuel compression ratio; however, knocking, which is a devastating and abnormal combustion phenomenon, occurs under critically constrained conditions in the development of high-efficiency engine [2]. This trade-off makes it difficult to achieve the theoretical maximum combustion efficiency in practical engines. Finding a balance between improved engine performance and knocking inhibition has thus become a perpetual challenge to the engine manufacturing industry and researchers.

Because end-gas auto-ignition is the first stage of knocking, whose subsequent development determines the knocking occurrence and intensity, in general, it can be concluded that knocking in SI engines is induced by auto-ignition occurring in the end gas [3,4], which has been extensively and comprehensively investigated. Many excellent studies have contributed to exploring the method of inhibiting such knocking, and several potential means have been discovered, including changing the flame propagation speed [5], increasing the in-cylinder turbulence [6,7], split injection strategies [8], octane number [9,10], and EGR (Exhaust Gas Recirculation) strategies [11]. For instance, Yang et al. [12] found a higher tumble rate can lead to the increase of flame speed through by facilitating the interaction between the fuel spray and air flow and the heat-mass transfer between the unburnt and burnt zone. Kim [13] studied the effects of hydrogen on a gasoline direct injection engine and found that hydrogen addition can inhibit the propensity of knocking combustion under high-load conditions because of its high flame velocity. However, the decelerated flame propagation velocity induced by cooler EGR [11] accompanied by reduced end-gas temperature could also mitigate knock occurrence. Yue et al. [14] found that increasing flame speed shows a negative impact on knock mitigation, but provides improvement on thermal efficiency by shortening the combustion duration. However, some research [15,16] shows that relatively low turbulence intensity gives the longer residence time for end-gas auto-ignition occurrence, thus knock is intensified. This contrast manifests that the underlying mechanism of the effects of flame propagation speed on auto-ignition is unclear.

In fact, there are disagreeing opinions among researchers regarding whether an increase in the flame speed is capable of inhibiting knocking. Kee et al. [5] developed a rapid compression/expansion device to explore the essential phenomenon of knocking. Their results indicate that increasing the laminar flame speed inhibits the knocking because a fast propagation decreases the time required for low-temperature reactions in the end gas. Hirooka et al. [17] believe that increasing the burn rate is also effective in improving the knocking characteristics. However, many studies have indicated the opposite [18,19]. For instance, Chen and Raine [19] proposed a multi-step adiabatic constant-volume zero-dimensional (MACZ) model to calculate the chemical reaction of an unburned air-fuel mixture and pointed out that increasing the burning rate promotes knocking through two factors, namely, “pre-dominant” steps and “post-dominant” steps. Furthermore, Yu et al. [20] conducted a 1D simulation regarding the effects of the flame propagation velocity on the end-gas auto-ignition in a constant volume combustion chamber by introducing artificial mass diffusivity. They found that increasing the flame propagation can suppress the knocking occurrence if the chamber size is sufficiently small. In our previous work [21], the knock phenomenon under the influence of different acceleration flame is investigated by conducting a series of 2D DNS (Direct Numerical Simulation) investigation. Three modes were found to exist, namely auto-ignition promoted by strong flame acceleration, auto-ignition suppressed by weak flame acceleration, and auto-ignition independent of flame acceleration. Such studies clearly show how our understanding of the effect of the flame propagation velocity has changed, whereas the knock mode transition from inhibition to promotion has not been understood, which is very important to suppress knock in SI engines.

It is generally accepted that turbulence intensity influences the end gas properties. Mastorakos et al. [22] conducted a two-dimensional direct numerical simulation on the auto-ignition of laminar and turbulent mixing layers. They found that the auto-ignition time in the turbulent flows is longer than the ignition delay time of homogeneous mixtures. Juan et al. performed an experimental investigation regarding the turbulence intensity on knock tendency in a SI engine. It was found that increased turbulence intensity increased the knocking tendency. Besides, the turbulent flame propagation investigations associated with pressure oscillation [23], flame-shock interaction [24], and flame acceleration [25] were widely conducted. Those work observed the auto-ignition process visually, yet the fundamental auto-ignition mechanism of how the turbulence influences the end gas auto-ignition is still less understood.

Therefore, the major objective of the present study is to comprehensively study the effects of the flame propagation velocity and turbulence intensity on the end-gas auto-ignition in a downsized

SI gasoline engine, as well as the pressure oscillation through a large eddy simulation coupling with a decoupling methodology. The SAGE solver coupling with a detailed chemistry mechanism of the PRF (Primary Reference Fuel) is employed to capture the detailed reaction process as the end-gas auto-ignition occurrence. Note that, using flame models such as G-equation model to mimic laminar flame comprise the ability to mutually decouple flame propagation and end-gas auto-ignition. By modifying the coefficient in the G-equation, the flame speed is changed. Consequently, a quantitative analysis regarding the effects of the flame propagation velocity on the knocking occurrence was conducted in this study. Furthermore, the turbulence intensity is achieved by rescaling the in-cylinder flow velocity. The effects are further understood in terms of the pressure wave, HCO, flame front velocity, and unburned temperature distributions. The present study will deliver valuable and new perspectives for inhibiting the knocking and improving the performance in SI gasoline engines.

The remainder of the present paper is structured as follows: The experimental setting is briefly presented in Section 2. The numerical settings including the LES equations, combustion model, numerical model, model validation, and parameter setting are provided in Section 2. The effects of the flame propagation velocity and turbulence are discussed in Section 3. Finally, the concluding remarks are given in Section 4. The model validation is presented in Appendix A.

2. Numerical Setting

2.1. Combustion Model

The G-equation-based turbulent combustion model [26] is utilized to capture the turbulent flame propagation in the partially pre-mixed combustions. SAGE solver coupling with detailed chemistry mechanism of the PRF [27] is used to capture the detailed reaction process as the end-gas auto-ignition occurrence. Here, a simple description of G-equation is listed below.

The G-equation is [28]:

$$\frac{\partial \tilde{G}}{\partial t} + (\tilde{\vec{v}}_f - \vec{v}_{vertex}) \cdot \nabla \tilde{G} = \frac{\bar{\rho}_u}{\bar{\rho}} s_t |\nabla \tilde{G}| - D_t \tilde{k}_M |\nabla \tilde{G}|, \quad (1)$$

where $\tilde{G}$ is the Favre-averaged G, $\tilde{\vec{v}}_f$ is the Favre mean bulk fluid velocity in the flame front, $\vec{v}_{vertex}$ is the mesh vertex velocity, $\bar{\rho}_u$ is unburned mixture density, $\bar{\rho}$ is the mean gas density of a turbulent flame, D_t is the turbulent diffusivity, $\tilde{k}_M$ is the mean flame curvature, and s_t is the turbulent flame speed.

Here, s_t is the function of the laminar flame speed (s_l), and is expressed as follows [28]:

$$s_t = s_l + v' \left\{ -\frac{a_4 b_3^2}{2b_1} Da + \left[\left(\frac{a_4 b_3^2}{2b_1} Da \right)^2 + a_4 b_3^2 Da \right]^{\frac{1}{2}} \right\}, \quad (2)$$

where v' is the turbulence intensity; a_4 , b_1 , and b_3 are constants; and Da is the Damköhler number, which establishes the relationship between the chemical kinetic and flame development. In the present work, a_4 , b_1 , and b_3 are optimized trying to well reproduce the combustion characteristic such as cylinder pressure and heat release rate.

To obtain the laminar flame speed, the Metghalchi and Kech correlation [29] is adopted in this study:

$$s_l = s_{l-ref} \left(\frac{T_u}{T_{u,ref}} \right)^\alpha \left(\frac{P}{P_{ref}} \right)^\beta (1 - 2.1Y_{dil}). \quad (3)$$

Here, T_u is the unburnt mixture temperature, $T_{u,ref}$ is 298.0 K, P is the unburnt mixture pressure, P_{ref} is 1.01 bar, Y_{dil} is the mass fraction of the dilution species, and α and β are the temperature and pressure exponents:

$$\alpha = 2.18 - 0.8(\phi - 1), \quad (4)$$

$$\beta = -0.16 - 0.22(\phi - 1), \quad (5)$$

where s_{l-ref} is obtained using the Gülder correlations [30]:

$$s_{l-ref} = \omega \phi^\eta \exp[-\xi(\phi - \sigma)^2]. \quad (6)$$

Here, ω , η , ξ , and σ are the modeling constant coefficients for an iso-octane–air mixture.

To reproduce the experimental and suitable length and time scales of laminar flames, the model coefficients are calibrated and optimized, as shown in Table 1. It can be seen from Figure 1 that, for primary reference fuels with octane numbers varying from 85 to 95, the laminar flame speeds are quite close under different equivalence ratios. It is reasonable to speculate PRF92 behaves a similar curve in the laminar flame speed—equivalence ratio diagram. Comparing with Güler line and Metghalchi line, we can conclude that by adopting the revised coefficients, agreement with the experimental data can be obtained.

Table 1. Fitting coefficients of the laminar flame speed.

	ω	η	ξ	σ	γ	β
Gülder	0.4658	−0.326	4.48	1.075	1.56	−0.22
Present work	0.35	0.1	4.5	1.075	1.8	−0.22

Figure 1. Comparison of the fitting curves and experimental data of laminar flame speed.

2.2. Numerical Models

The 3D methodology of a LES coupled with a G-equation and a chemical kinetic model for the PRF oxidation in the CONVERGE CFD code is applied to the simulation used in this study. The reacting flow problems are described in terms of the mass, energy, species conservation, and the Navier–Stokes equations [31–33]. The detailed numerical models can be found in Ref. [34–36]. The geometry model, which consists of a combustion chamber, an inlet port, and an outlet port, together with its grid splitting, can be found in Figure 2. The ignition process is initiated by a spark located opposite the spray, which is supposed to ignite a flame core at ST −18. A base grid size of 1 mm is utilized, with a fixed embedding around the spark plug and spray to meet the required mesh resolution. Meanwhile, an adaptive mesh refinement (AMR) is adopted. During combustion, the average grid size in the flame front is 0.5 mm, and is on the order of 0.125 mm around the spark plug during the spark process and 0.25 mm near the spray during the injection. A maximum of 4 million cells is achieved. Note that, according to a

previous study, the present grid resolution can predict the occurrence of super-knocking [37]. The time step adjusts itself according to the CFL (Courant–Friedrichs–Lewy) number, which varies from 1×10^{-8} to 1×10^{-6} s.

Figure 2. Schematic of the model structure and grid splitting.

2.3. Different Case Settings

2.3.1. Effects of Flame Propagation Velocity

In practical engines, the flame propagation velocity is physically under the joint action of the laminar flame speed, turbulent flame speed, and in-cylinder turbulent flow. Hence, it is tricky to directly change flame propagation velocity. Keeping in mind that turbulent flame speed is a function of laminar flame speed and turbulence intensity as Equation (3) implied, we find a solution. Furthermore, according to an Equation (6) proposed by Gülder [30], the laminar flame speed has a linear relationship with coefficient ω , which means that a monotonically increasing of laminar flame speed would be observed when other parameters are identical. Thus, we can decouple the flame velocity from the end-gas auto-ignition. Table 2 lists the operating parameters for studying the effects of flame propagation velocities.

Table 2. Operating parameters.

Parameter	Value
Onset of calculation time	−30 CAD aTDC
Spark timing	−18 CAD aTDC (ST-18)
Baseline case: ω	0.36
Cases: ω	0.4, 0.5, 0.6, 0.7, 0.8

2.3.2. Effects of Turbulence Intensity

Figure 3 illustrates the variations of the cold flow at −18 CAD aTDC (after top dead center) and TDC after amplifying the flow velocity at −30 CAD aTDC. It can be seen that present setting has the ability to capture the turbulence dissipation as the vortex structure breaks up and disappears over time. The vortex structure becomes more obvious and complicated as u/u_0 increases, and remains to the TDC. These results indicate that the method of amplifying the flow velocity enhances the in-cylinder turbulence intensity. The evolution of the TKE (Turbulent kinetic energy) after scaling the flow velocity

at different times is illustrated in Figure 4. It can be seen that the TKE increases first as the flow velocity increases, but subsequently decreases owing to the viscous dissipation. However, the TKE maintains a proportional relationship with u/u_0 . Figure 5 shows the variation of TKE with u/u_0 at -18 CAD (spark timing) and TDC. At -18 CAD aTDC, the TKE and u/u_0 basically exhibit a linearly positive relationship regardless of the timing of the scaling; however, the situation at the TDC is different. At the TDC, owing to viscous dissipation, the attenuation of TKE is positively related to the flow velocity and mapping timing. For instance, in the case of map -120 CAD and map -60 CAD, the TKE is not linearly related to u/u_0 , whereas in the case of map -30 , this linear relationship remains well owing to the lesser decay. Therefore, map -30 CAD is utilized. Detailed operating parameters can be found in Table 3.

Figure 3. Evolution of different initial velocity fields.

Figure 4. Evolution of averaged TKE after scaling the flow velocity at different times.

Figure 5. Values of TKE for different u/u_0 at the instant of (a) -18 CAD aTDC and (b) TDC.

Table 3. Operating parameters in the analysis of the effects of turbulence intensity.

Parameters	Value
Onset of calculation timing	-30 CAD aTDC
Sparking timing	-18 CAD aTDC (ST-18)
Base case: u/u_0	1.0
Ratios: u/u_0	1.5, 2.0, 2.5, 3.0, 4.0

3. Results and Discussion

3.1. Effects of Flame Propagation Velocity

3.1.1. Analysis of Cylinder Pressure and HRR

Figure 6 demonstrates the pressure profiles and filtered pressure oscillations affected by different laminar flame speeds. In addition, Figure 7 demonstrates the MAPO (Maximum Amplitude Pressure Oscillation) and onset of auto-ignition with different flame speeds. The peak pressure and amplitude of the pressure oscillation first increase and then decrease as increasing the flame propagation velocity. However, the onset of auto-ignition advances as increasing the flame propagation velocity. The strongest knocking intensity with a peak pressure of 35 MPa appears at $\omega = 0.5$, whereas another pressure oscillation of high amplitude with a peak value of approximately 25 MPa appears at $\omega = 0.6$. Thus, it can be implied that super-knocking occurs under both conditions. A further increase in the flame propagation velocity leads to a cliff-like decrease in the pressure profile and knocking intensity; for instance, the pressure oscillation amplitude is below 0.5 MPa at $\omega = 0.7$ and $\omega = 0.8$, which means the knocking or pressure oscillation disappears. This in-depth mechanism can be demonstrated through 3D images, as discussed later. The evolutions of HRR (Heat Release Rate) and BMF (burned mass fraction) with different flame propagation speeds are plotted in Figure 8a. At $\omega = 0.36$ and $\omega = 0.4$, the profile of the HRR exhibits a bimodal shape. Meanwhile, as the flame propagation speed increases, the onset of AI (auto ignition) advances and the peak value of HRR increases, whereas the heat release duration decreases. These results indicate that two individual AIs occur in an unburned mixture. The higher the flame speed is, the closer is the overall combustion process to the TDC, resulting in higher average temperature and pressure. As a result, auto-ignition in the end-gas region is prone to occur. In addition, higher thermodynamics provides favorable conditions for a higher combustion rate after the occurrence of AI. However, pressure oscillation is weak. Furthermore, a unimodal shape of HRR with higher peak pressure is exhibited with an increase in the flame propagation speed. The unimodal shape of HRR implies that an individual hot spot or auto-ignition occurs in the unburned

gas. Consequently, the auto-ignition flame completely consumes the residual unburned gas in the end-gas region at a speed close to the CJ velocity.

Figure 6. Pressure profiles and filtered pressure oscillations with different flame velocities.

Figure 7. MAPO and onset of auto-ignition with different flame velocities.

(a) HRR and BMF profiles

(b) HRR at $\omega = 0.36$ (c) HRR at $\omega = 0.5$

Figure 8. (a) HRR and BMF profiles with different flame velocities and amplified HRR profile of (b) $\omega = 0.36$ and (c) $\omega = 0.5$.

To clearly demonstrate the heat release process under different conditions, the HRR profiles at $\omega = 0.36$ and $\omega = 0.5$ are amplified, as shown in Figure 8b,c, respectively. At $\omega = 0.36$, the HRR increases gradually before the onset of the first AI, after which it experiences a steep lift. Together with the subsequent decrease, the enclosed yellow area can be plotted to represent the heat release process by the first AI flame. At 13.8 CAD aTDC, the HRR increases again with a fast growth rate, which indicates the occurrence of a second AI. Similarly, the green area represents the heat released by the second AI flame. Durations of 2 CAD aTDC and 1.8 CAD aTDC for the two AIs can be observed. For the case at $\omega = 0.5$, a single peak of HRR 4-times that of HRR at $\omega = 0.36$ is observed, whereas the fast heat release duration is approximately half of the heat release for two AIs at $\omega = 0.36$. No obvious peak in the HRR is observed because of the absence of the AI when the flame propagation speed is further increased by increasing the coefficient to $\omega = 0.7$ and $\omega = 0.8$. Furthermore, the BMF diagram reveals that the mass fraction of unburned gas consumed by the AI decreases gradually as the flame propagation speed increases. For instance, 97.5% of the mixture is consumed by the main flame at $\omega = 0.7$, whereas at $\omega = 0.8$, the main flame has already swept the entire combustion chamber before auto-ignition occurs owing to a very fast flame propagation speed, resulting in the absence of auto-ignition at $\omega = 0.8$. Slight pressure oscillations can still be observed under the two conditions. It is worth mentioning that Rober et al. [38] presented that the pressure wave intensity is proportional to the burned mass by AI, and they also suggested that AI location and the coupling between the pressure wave and the AI flame propagation are also probably factors to control knock intensity. However, the present results demonstrate the non-monotonic relationship between the flame propagation velocity or BMF and the knock intensity. Such phenomena can be clearly explained by the detailed flame propagation process under different conditions, as shown in the latter figures.

To summarize, increasing the flame propagation velocity will first strengthen the knocking intensity and then weaken it. There are two aspects to this. On the one hand, a higher flame velocity results in an increase of the heat release rate in the cylinder, consequently obtaining quicker increases of temperature and pressure at the end-gas region. Therefore, the ignition delay time of the unburned end-gas mixture is shortened, which can promote a hot-spot formation or the occurrence of auto-ignition. On the other hand, the higher the flame propagation velocity is, the shorter the time required for the main flame propagating from the spark to the end-wall. If all fuel-air mixtures are consumed by the main flame before an auto-ignition occurs, the auto-ignition will not appear. The competitive relationship between the flame propagation velocity and end-gas auto-ignition brings about a non-monotonic relationship between the flame propagation speed and knocking intensity. Meanwhile, the intensity of the knocking does not depend solely on the flame propagation velocity, but also on the mass of the unburned mixture when auto-ignition occurs. The most intense knocking is observed when both the flame propagation velocity and mass of the unburned mixture are significant. However, a sufficiently high flame propagation velocity will decrease the knocking intensity as a result of the absence of the AI or an insufficient unburned mixture as auto-ignition occurrence. This phenomenon is consistent with the 1D DNS results from Yu et al. [20].

3.1.2. Analysis of Combustion Process

To further study the influence of the different flame velocities on the end-gas auto-ignition and pressure oscillation, the effects of the flame propagation velocities at $\omega = 0.5$ and $\omega = 0.8$ are considered.

(1). Combustion characteristics at $\omega = 0.5$

Figure 9 shows the evolution of the main flame propagation and end-gas auto-ignition at $\omega = 0.5$. Noted that, the isosurface for $G = 0$, marked by the red color, indicates the main flame front [28]. The onset of an auto-ignition is localized by the isosurface of HCO with a mass fraction of 3.0 ppm [39], and the isosurface of the unburned mixture at a temperature of 1600 K at the end-gas region represents the flame front induced through an auto-ignition. The distribution of the local pressure fluctuation (ΔP), which is calculated by the difference between the local pressure and the average pressure in the cylinder,

is also demonstrated. An obvious auto-ignition spot appears at 4.5 CAD aTDC near the bottom left wall under a large accumulation of HCO owing to low-temperature reactions, which is immediately consumed by the subsequent high-temperature reactions, forming a stable flame. Under this condition, although only one auto-ignition spot occurs, the mutual interaction between the developed flame front induced by AI and a pressure wave leads to a much higher explosive pressure, which finally results in violent knocking combustion. Figure 10 shows the distribution of the pressure fluctuation, HCO, and unburned temperature (UT) on a horizontal plane with $z = -3$ mm. The purple line indicates the main flame front by the contour of $G = 0$. It can be clearly seen from the pressure fluctuation that the flame front generated by the AI on the right side is at the same position as the pressure wave during the period of 4.9 CAD to 5.1 CAD aTDC. In addition, the pressure fluctuation at the flame front achieves the peak value. The flame propagation speed on the right side is approximately 1.7 km/s, which is close to the Chapman–Jouguet (CJ) detonation velocity and confirms the occurrence of a detonation here. The present result agrees with the result by Robert et al. [37], which confirmed the hypothesis proposed in the previous works [40] that super-knock is characterized by a deflagration to detonation (DDT). In addition, recently, the super-knock with DDT phenomenon also can be distinctly observed by an optically rapid compression machine (RCM) [41]. The present flame propagation as shown in Figure 9 is similar to the detonation propagation in [41].

Figure 9. Evolution of main flame propagation and end-gas auto-ignition at $\omega = 0.5$ by 3D isosurfaces of $G = 0$ and mass fraction of HCO = 3 ppm; the background color indicates the pressure evolution.

Figure 10. Evolution of ΔP , mass fraction of HCO, and unburned temperature after the initial auto-ignition at $\omega = 0.5$.

In [37], a circular 1D profile is extracted from the periphery of the combustion chamber to quantitatively analyze the cause of knock mechanism by comparing the pressure profile and auto-ignition reaction rate at every angular degree. This method describes the super-knocking mechanism well. Therefore, to further investigate the coupling between the flame and pressure wave, a path, as shown in Figure 11, is applied by extracting the 1D profiles of the pressure, unburned temperature, and mass fraction of HCO, and the profiles along with 2D images are illustrated in Figure 12. It can be seen from the 4.7 CAD aTDC to 4.8 CAD aTDC that a large amount of HCO is generated on the right side of the auto-ignition flame, indicating that sequential AIs occur in the region. During this period, the AI flame propagates with a deflagration velocity of approximately 730 m/s, exceeding the local acoustic speed. In addition, at 4.8 CAD aTDC, the pressure peak at the right side of the auto-ignition flame clearly increases. At this time, the auto-ignition flame speed is approximately 1.3 km/s, which is slightly lower than the CJ velocity. Owing to the fast heat release, the intensity of the pressure wave continues to enhance, and the pressure wave reaches a peak of 28 MPa at 4.9 CAD aTDC. It should be noted that, at this time, a coupling between the auto-ignition flame and pressure wave is formed, and the combustion mode completes the transitions from auto-ignition to a deflagration flame to detonation, which consequently generates the occurrence of super-knocking. This process is consistent with the work in [37]. Next, the subsequent detonation combustion wave proceeds to consume the unburned gas at a speed of 1.7 km/s, and the maximum pressure reaches 31 MPa. It is not until the unburned mixture on the left side of the flame is completely consumed at 5.1 CAD aTDC that the pressure wave detaches from the flame front, indicating the end of the detonation combustion. On the left side of the auto-ignition flame, the propagation speed remains at approximately 240 m/s, which is clearly inferior to the speed of the pressure wave, and thus a coupling between the auto-ignition flame and pressure wave does not appear here.

Figure 11. Schematic of trace from which the 1D profile is extracted.

(2). Combustion characteristics at $\omega = 0.8$

Figure 13 demonstrates the evolution of the main flame propagation and end-gas auto-ignition at $\omega = 0.8$. Under this condition, the auto-ignition does not occur. As the figure indicates, the main flame has already swept the entire combustion chamber at -1 CAD aTDC, leading to the suppression of the end-gas AI. Similar results can be concluded from the distribution of HCO and UT. No obvious accumulation of HCO or an increase of UT occurs, as shown in Figure 14. However, the pressure oscillation with an amplitude of approximately 3 bar can still be observed from the distribution of the pressure fluctuation. This phenomenon implies that the in-cylinder pressure wave oscillation can not only be induced by auto-ignition, but can also be caused by a fast heat release or accelerated flame if it is sufficiently fast to induce a local pressure increase, which was confirmed in previous studies [42–44]. Meanwhile, it can be seen that multiple pressure waves are generated during the flame propagation. The pressure waves continuously compress the unburned mixture, increasing the local temperature and pressure, which in turn enhances the flame propagation. It should be noted that the pressure oscillation induced by the main flame is far lower than that by the end-gas auto-ignition. Therefore, knocking can be inhibited by increasing the flame propagation velocity; however, it can be reasonably

predicted that a further increase in the flame velocity will cause higher pressure oscillations owing to the increase in HRR. Overall, for a quickly accelerating flame, the interactions between the flame, compress wave, and auto-ignition dominate the occurrence of knocking combustion.

Figure 12. Evolution of 2D pattern of ΔP in the horizontal cross-section (left), pressure, unburned temperature, and mass fraction of HCO on the 1D profile (middle) and 2D pattern of unburned temperature in the horizontal cross-section (right) under the condition of $\omega = 0.5$.

Figure 13. Evolution of 3D in-cylinder combustion process at $\omega = 0.8$.

Figure 14. Evolution of ΔP , mass fraction of HCO, and unburned temperature after the initial auto-ignition at $\omega = 0.8$.

3.2. Effects of Turbulence Intensity

Unlike the effects of the turbulent flame velocity on the end-gas auto-ignition and knocking occurrence, increasing the turbulence intensity must simultaneously change the flame propagation and thermodynamic state involving the temperature and compositions in the end-gas region. Here, the effects of the turbulence intensity by changing the flow velocity on the end-gas auto-ignition and pressure oscillation are determined.

3.2.1. Analysis of Cylinder Pressure and HRR

Figure 15 shows the pressure profiles and filtered pressure oscillations with different turbulence intensities. Similar to the effects of the flame velocity on the knocking intensity, a non-monotonic relationship between the turbulence intensity and the pressure oscillation is observed from the flame-turbulence interaction. The combustion phenomenon is consistent with the results obtained from a 1D simulation described in previous studies [45,46]. On the one hand, the increased turbulence intensity can promote important intermediate radicals and heat dispersions, which finally retards the onset of the AI and reduces the AI kernel size [47]. On the other hand, increasing the turbulence intensity can also increase the wrinkled flame surface and burning rate, which results in an increase in the flame propagation velocity. As discussed above, the effects of the flame propagation speed on the end-gas auto-ignition are also non-monotonic. Both causes will ultimately influence the knocking

tendency and intensity. However, the previous studies neglected the effects of flame propagation and compression wave.

Figure 15. Pressure traces and filtered pressure oscillations with different turbulence intensities.

It is worth noting that the MAPO under enhanced turbulence intensity conditions is generally lower than that under the flame speed cases. In addition, none of the MAPOs here exceeds 1.5 MPa, as shown in Figure 16. The more intense the turbulence is, the faster the main flame propagates, which promotes the pressure increase and advances the onset of the pressure oscillation. As a result, the mean in-cylinder pressure is also high as a pressure oscillation occurs. Compared to the effect of the flame speed, the effect of the turbulence on the pressure oscillation is more complicated, as discussed above. Therefore, to further decouple the flame acceleration from the end gas auto-ignition, applying the mean combustion rate (BMF when auto-ignition occurs is divided by the difference of auto-ignition timing and spark timing) before the auto-ignition occurrence is proposed to indicate the main flame propagation speed. Similarly, the effect of different flame speeds on the end-gas auto-ignition is also determined using the same method as a comparison. Figure 17 demonstrates the relationship between the MAPO and the combustion rate before the AI in terms of the increase in flame speed and an increase in turbulence intensity, respectively. By comparison, under the same mean combustion rate, the MAPO obtained by changing the turbulence intensity is far lower than that obtained by increasing the flame speed, which indicates that increasing the turbulence can effectively suppress the auto-ignition.

Figure 16. MAPO and onset of auto-ignition with different turbulence intensities.

Figure 17. Relationship between MAPO and the combustion rate before auto-ignition as increasing the flame speed and increasing the turbulence intensity.

The HRR and BMF profiles at different turbulent intensities are plotted in Figure 18. The bimodal curve of the HRR reveals the occurrence of two individual AIs. As the turbulence intensity increases, the first peak by the first AI is gradually inhibited, whereas the second peak first increases and then decreases. This indicates that the turbulence first leads to a more homogenous reactivity and an increase in the thermodynamic state in unburned gas for the second AI spot. Thus, the heat release rate increases. In contrast, a further increase of the turbulence intensity will increase the propagation velocity of the main flame as well as the ignition delay of the end gas, which means a reduction of the unburned mixture when an auto-ignition occurs. As a result, the HRR gradually decreases. For instance, approximately 97.1% of the fuel-air mixture is consumed by the main flame when auto-ignition occurs at $u/u_0 = 4.0$, and therefore the amplitude of the pressure oscillation under this condition is only 0.27 MPa, which is even smaller than the case of $\omega = 0.8$ where no auto-ignition is observed.

Figure 18. HRR and BMF curves with different turbulence intensities.

3.2.2. Analysis of Combustion Process

The profile of the HRR under different turbulence intensities can be divided into two categories. The cases of $u/u_0 = 1.5, 2.0$, and 2.5 share similar bimodal curves of the HRR, which means they have a similar combustion process. For $u/u_0 = 3.0$ and 4.0 , the curves of the HRR are unimodal evolutions. Based on this, the two turbulence intensities at $u/u_0 = 1.5$ and $u/u_0 = 4.0$ are adopted to analyze the in-cylinder combustion process affected by the turbulence intensity.

(1). Combustion characteristics at $u/u_0 = 1.5$

Figure 19 shows the in-cylinder combustion characteristics for $u/u_0 = 1.5$. In addition, for the evolution of ΔP , the mass fraction of the HCO and the unburned temperature at $u/u_0 = 1.5$ are illustrated in Figure 20. As the figure indicates, auto-ignition first occurs near the bottom left wall at 7.3 CAD aTDC with a large amount of HCO accumulated around the initial auto-ignition kernel, denoting the occurrence of sequential auto-ignitions in this region. The fast heat release generated by the AI results in a local pressure increase and triggers the pressure waves. However, the pressure waves have a higher propagation velocity than the AI flame speed. In addition, the limited mass of the unburned mixture around the AI spots further prevents the coupling between the flame and pressure wave, which does not lead to a strong pressure oscillation according to a previous study. Affected by the compression effects of both the main flame and the auto-ignition flame, a second auto-ignition appears on the right side of the combustion chamber at 8.3 CAD aTDC. The in-cylinder pressure and temperature are further increased compared to the first auto-ignition, which leads to a more intense heat release, generating stronger pressure waves. As shown in [45,46], the increased turbulence intensity has the capability of delaying the onset of the AI formation and shrinks the kernel size at the onset of AI because of turbulence stirring and subsequently the enhance localized energy and radicals dissipation, which results in the decrease of unburned mixture amount if AI occurs. The in-depth analysis of the similar work is confirmed by the work of Wu et al. [48]. However, as pointed out by Wei et al. [46], the increased turbulence stirring results in the increases of mean temperature and pressure of the unburnt mixture. Furthermore, the increased turbulence also can promote flame propagation induced by the AI due to increasing the turbulent flame surface. As a consequence, although the remaining unburned mixture when auto-ignition occurs is less than that for the baseline case, noted that, the mean thermodynamic states involving the temperature and pressure are higher, which introduces a more intense heat release and strengthens the pressure oscillation ultimately. The present result indicates that the thermodynamic states dominate the combustion intensity and not only the unburned mixture mass.

Figure 19. Evolution of 3D in-cylinder combustion process at $u/u_0 = 1.5$.

Figure 20. Evolution of ΔP , mass fraction of HCO, and unburned temperature after the initial auto-ignition at $u/u_0 = 1.5$.

(2). Combustion characteristics at $u/u_0 = 4.0$

Figure 21 demonstrates the evolution of the main flame, auto-ignition flame, and pressure wave based on 2D images as auto-ignition occurs, respectively. Only one auto-ignition is observed on the right side of the combustion chamber where a second AI was found in previous cases. The absence of AI in the first AI position mentioned above can be attributed to the increase in flame propagation speed and the dissipation of heat and intermediate radicals generated by low-temperature reactions around the AI kernel. These impacts substantially retard the ignition delay, resulting in the consumption of the unburned mixture by the main flame before auto-ignition. Compared to the case of $u/u_0 = 1.5$, the increased flame speed dominates the combustion process and suppresses the end-gas auto-ignition due to the distinct effect of enhanced turbulence intensity. At 1.5 CAD aTDC, the AI occurs with the consumption of the remaining unburned gas during 0.4 CAD. Limited by the mass of the available unburned mixture, the auto-ignition does not produce strong pressure oscillations. Note that, under this condition, a pressure wave with a slight intensity can be observed at 1.3 CAD aTDC, even before the occurrence of auto-ignition. This phenomenon can be explained by the intense combustion process and fast heat release rate induced by the fast propagation speed of the main flame.

Figure 21. Evolution of ΔP , mass fraction of HCO, and unburned temperature after the initial auto-ignition at $u/u_0 = 4.0$.

4. Conclusions

The major objective of the present work is to investigate the effects of the flame propagation velocity and turbulence intensity on the end-gas auto-ignition as well as pressure oscillation through an LES and a decoupling methodology applied in a downsized SI gasoline engine. The mechanisms of end-gas auto-ignition and a strong pressure oscillation were qualitatively analyzed. In this work, it should be noted that, based on the G-equation model and SAGE solver, a decoupling of the relationship of the flame propagation velocity and the thermodynamics of the end-gas mixture was achieved. A validation of the pressure evolution and HRR was conducted under different combustion conditions, and the results indicate that the present model is capable of capturing the combustion characteristics under wide operating conditions. The following remarkable results were found:

1. The knocking intensity or maximum pressure oscillation, as well as the MAPO, first experiences an increase and then a decrease as the flame propagation speed increases, which presents a non-monotonic relationship with the flame propagation velocity. The competitive relationship between the flame propagation velocity and the ignition delay of the end gas is responsible for this phenomenon. The higher flame speed leads to an increase in the heat release rate in the cylinder, and consequently, quicker increases in the temperature and pressure of the unburned end-gas mixture are obtained, leading to an end-gas auto-ignition. However, the sufficiently high propagation velocity of the flame will reduce the mass fraction of the unburned mixture consumed by the AI, thus ultimately decreasing the knocking intensity. Furthermore, the coupling of the pressure wave and AI flame front results in super-knocking with a maximum peak in pressure of 31 MPa.
2. The non-monotonic relationship between the end-gas auto-ignition and turbulence intensity was also observed. On the one hand, an increased turbulence intensity can accelerate the dissipation of the key intermediate radicals and heat energy, which finally retards the AI formation and shrinks the kernel size of the AI. On the other hand, increasing the turbulence intensity can also wrinkle the flame surface and increase the burning rate, which results in an increase in the flame propagation velocity. It can be concluded that the turbulence intensity has a more complicated effect on the knocking compared to the flame propagation velocity.
3. The evolutions of the main flame propagation velocity and end-gas auto-ignition and a profile of the HRR revealed that the influence of both the flame speed and the turbulence intensity can lead to two different combustion modes. The unimodal and bimodal shapes of the heat release rate are obtained, which is strongly dependent on the main flame propagation velocity, unburned mixture mass, and thermodynamic state in the end-gas region.

In the present work, the LES method is selected to simulate the turbulence evolution. However, the present work only focuses on the quantitative analysis of effects of turbulence intensity and flame propagation velocity on the super-knock by conducting a series of parameter studies under given settings conditions, thus the effects of the cycle-to-cycle cannot be achieved, which is unignorable in practical engines. Therefore, the cycle-to-cycle variations should be taken into consideration, and the simulation should be expanded to multi-cycles conditions. Meanwhile, effects of temperature and reactivity inhomogeneities on knock combustion are supposed to be conducted as those two parameters are closely related to the knock phenomenon in practical engines.

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Abbreviations

aTDC	after top dead center
AMR	adaptive mesh refine
AI	auto-ignition
BMF	burned mass fraction
CFD	computational fluid dynamics
CFL	Courant–Friedrichs–Lewy
CJ	Chapman–Jouguet
DNS	direct numerical simulation
DDT	deflagration to detonation transition
FFT	fast Fourier transform
GDI	gasoline direct injection
HCCI	homogeneous charge compression ignition
HRR	heat release rate
KH	Kelvin–Helmholtz instability
LEM	linear Eddy model
LES	large Eddy simulation
MAPO	maximum amplitude of pressure oscillation
RT	Rayleigh–Taylor instability
PRF	primary reference fuels
SI	spark ignition
RCM	rapid compression machine
UT	unburned temperature
TKE	turbulent kinetic energy

Appendix A

Model Validation

In our previous works [34–36], we have comprehensively validated the present models in terms of pressure profiles and heat release rate. The numerical pressure evolution agrees well with the experimental results, both in ST-10 case and ST-18 cases. Noted that, our present numerical model not only captures the knocking phenomenon but also captures the combustion mode transition as spark timing from the ST-10 to ST-18. It should be noted that in the present paper, we only focus on the quantitative analysis of effects of turbulence intensity and the flame propagation velocity on

the super-knock through a series of given settings as a fundamental study of knocking combustion, and thus the effects of the cycle-to-cycle variations cannot be achieved in the present model.

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