Initiation of detonation in iso-octane/air mixture under high pressure and temperature condition in closed cylinder

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1 Introduction

In recent decade, high boost and direct injection hold the potential of enhancing power density and fuel economy in gasoline engines. The development, however, has been challenged by the occurrence of a new engine knock mode, called super-knock [1], unwanted pre-ignition [2], mega knock [3], low-speed pre-ignition (LSPI) [4] or deto-knock [5], in highly boosted gasoline engines at the low-speed high-load operating regime. Super-knock can lead to very high peak pressure and pressure oscillation, in some cases, the peak pressure could exceed 200 bar and the amplitude of pressure oscillation over 100 bar [5], which could damage the engine in one engine cycle. Recent studies have indicated that super-knock may relate to detonation [5][6][7][8].

In terms of engine knock in piston engines, pioneers in this field of science used original technique for photographing end gas auto-ignition, fast flames and detonations. Detonations dated back to 30s to 50s of the last century. Sokolik and Voinov [9] reported an observation of detonation wave in an optical engine using streak photography. The results showed that the flame propagated at the speed less than 20 m/s in the combustion chamber, and then traveled the remaining space at a velocity of the order of 2,000 m/s. Miller [10] presented the evidence on the observation of detonation wave in the combustion chamber using schlieren photography at the frame rate of 40,000 and 200,000 fps. Male [11] used higher frame rate (500,000 fps) and found that end gas explosive detonation reaction might be composed of many individual detonation reactions.

In terms of detonation in the reactive gas, Zel'dovich [12] classified the autoignition ("spontaneous propagation") into four modes: 1) near thermal explosion without shock wave, 2) detonation propagating supersonically, 3) deflagration propagating subsonically, and 4) normal flame propagating by molecular diffusive and conductive mechanisms. Later, other researchers extended Zel'dovich's work using either H2/CO/Air reaction [13][14] or large hydrocarbon chemistry [5][8]. Gu and Bradley [10] extended the auto-ignition theory of temperature gradient. They demonstrated five propagation modes of autoignition front:

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thermal explosion, supersonic autoignitive deflagration, developing and developed detonation, subsonic autoignitive deflagration, and conventional laminar burning deflagration. To consider the large hydrocarbon fuels with negative temperature coefficient (NTC) behavior, Dai and Chen et al [8] carried out numerical experiments on reaction front propagation in n-heptane/air mixture with temperature gradient. It was found that shock compression of the mixture between the deflagration wave and the leading shock wave produces an additional ignition kernel, which determines the autoignition modes. To consider the high-octane fuel under highly boosted gasoline engine conditions, Wang and Liu et al [5] carried out both experimental investigation and numerical simulation. It was found hotspot in the mixture at typical near top dead center (TDC) pressure and temperature condition can only induce deflagration. Hot-spot in the unburned end-gas mixture at temperature and pressure conditions above “deto-curve” may induce detonation.

From the above analysis, although the theoretical investigations and engine experimental data indicate that super-knock may relate to detonation, no direct visualization of detonation was observed during super-knock in optical engines. Compared to the optical engine, the rapid compression machine (RCM) can work under much higher pressure and provides excellent optical accessibility. Using RCM, Wang and Qi et al [15] captured the events of pre-ignition and super-knock under high temperature and high pressure by simultaneous high-speed direct photography and pressure measurement. The results demonstrate that the mechanism of super-knock is constituted by hotspot-induced deflagration to detonation followed by high-pressure oscillation (DDP).

From the above review, it can be concluded that the combustion characteristics of super-knock are not fully understood and the process from deflagration to detonation is in particular poorly understood, even though various studies, including numerical simulation and optical measurements, have been carried out. The objective of this paper is to further reveal the initiation of detonation under engine-like conditions. In this work, the most representative detonation mode in iso-octane/air mixtures under high temperature and high pressure condition in a closed cylinder was detailed investigated.

2. Experimental setup

2.1 Rapid compression machine

The experiments were conducted using an RCM at Tsinghua University. The detailed information about the RCM can be found in Ref. [16]. A quartz end-window was used to allow optical access to the entire combustion chamber in axial direction. The pressure was measured using a flush mounted piezoelectric sensor (Kistler 6125C) and a charge amplifier (Kistler 5018A). The spark plug (Denso K20R) was mounted at the opposite side of the pressure sensor with electrodes located on the center of the combustion chamber. The detailed information about optical and data acquisition can be found in Ref. [12].

2.2 Test conditions

In this study, iso-octane (>99%) was used as the fuel. Ultra-high purity grade nitrogen (>99.999%) and oxygen (>99.995%) composed the rest of the test mixture. The equivalence ratio of the mixture is 1 with inert nitrogen to oxygen ratio of 3.76, i.e. the mole ratio of iso-octane : oxygen : nitrogen is 1:12.5:47. The mixture was prepared using a dedicated stainless steel mixing tank at room temperature (302 K).

The experiments were conducted at three compression ratios, 9.8, 12.2 and 15.5, which cover the range of the in-use modern production boosted engines. For the safety purpose, the targeted maximum pressure at the end of RCM compression was limited to 30 bar. All the RCM tests were conducted at room temperature (302 K). Both spark ignition (SI) and compression ignition (CI) combustion tests were conducted. Four detonation initiation modes were observed during the study. In this paper, only the most frequently observed mode (shock wave reflection induced detonation, (SWRID)) as shown in Table 1 is presented due to the page limitation.

Table 1. Experimental Condition of the SWRID.

CR	Condition at the end of compression		Condition right before the start of detonation			
	p [bar]	T [K]	p_0 [bar]	T_0 [K]	Local sound speed (m/s)	C-J speed (m/s)
9.8	20	641	63.054	824.11	541	1840

3. Results and discussion

Figure 1 presents the pressure trace of SWRID mode. Time 0 represents the time of spark firing, which initiates flame propagation causing slow pressure rise. At about 10.95 ms, sudden pressure rise and pressure oscillation were observed. In this case, the highest pressure oscillation amplitude is about 50 bar. Since Δp of the maximum permitted knock intensity is 5 bar for SI engine in general, this is a typical super-knock according to the knock intensity (Δp > 50 bar) defined in Ref. [5] based on experimental data statistics and combustion parameter calculations.

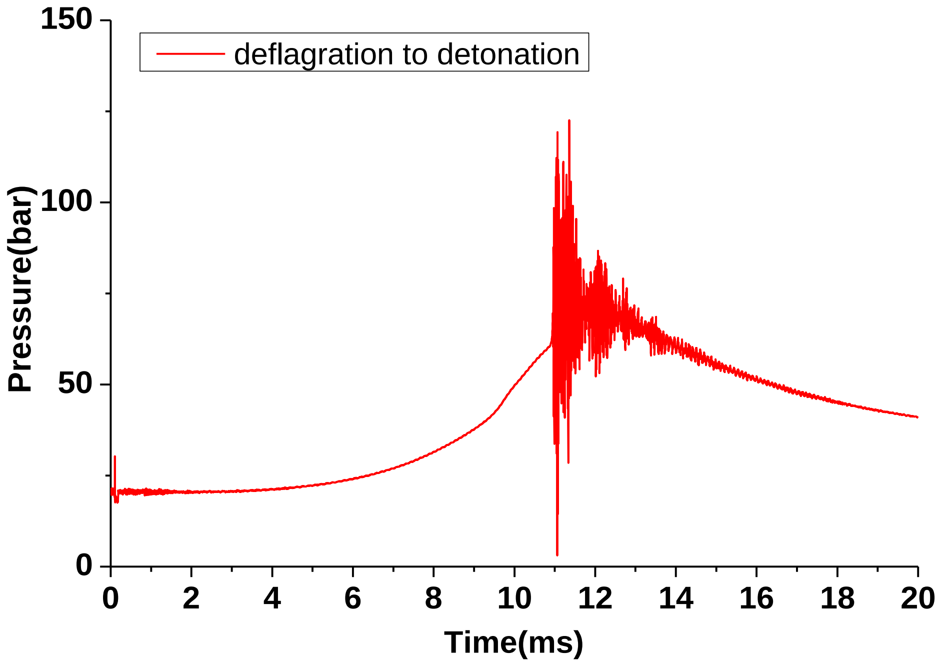
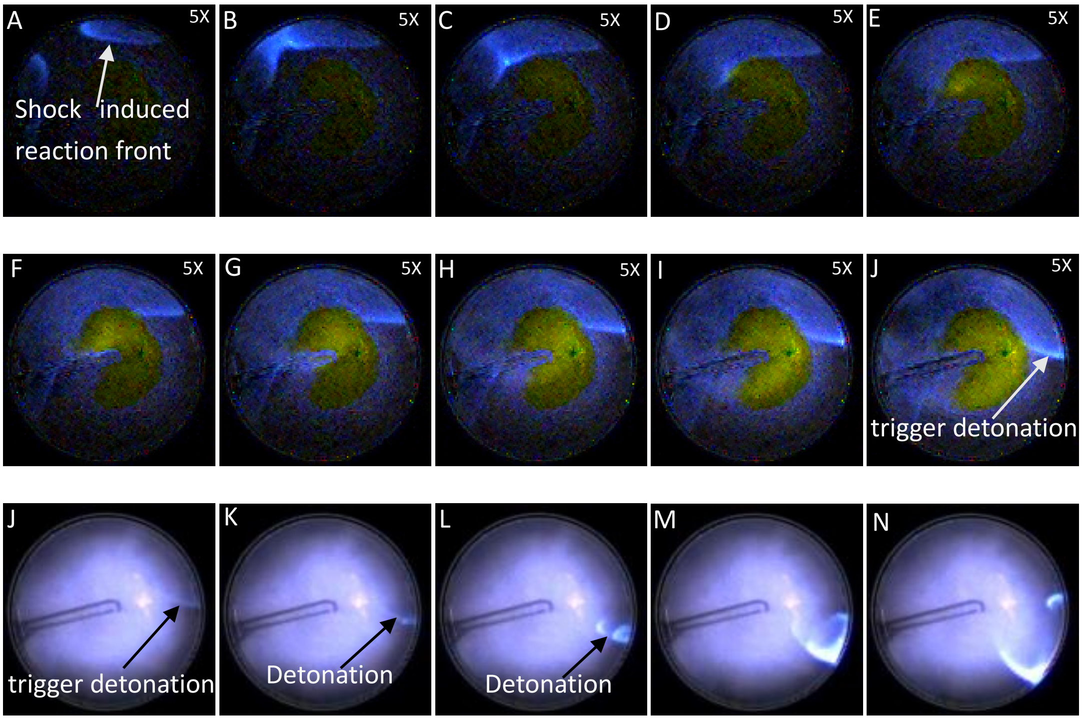


Figure 1. Pressure traces from deflagration to detonation

Figure 2 shows twenty consecutive high speed images of SWRID. Figure 3 presents propagation paths of the wave before and after detonation. The black solid lines represent the wave front of the corresponding images. At the time of Image A, two autoignitions occur almost simultaneously on the top and the left side of the combustion chamber. Two sharp and smooth waves were formed due to the autoignition and propagate into the unburned mixture. Note, the yellowish color in the center of the combustion represents the burned mixture due to the spark initiated flame propagation. Blue light emissions were observed for the gas mixture behind the waves, indicating chemical reactions. Based on the blue color intensity, the autoignition on the top of the combustion chamber is stronger. Thus the following discussion will be focusing on the combustion sequence induced due to the top autoignition.

The average wave speed along Paths 1 and 2 (shown in Figure 3a) are about 842 and 1052 m/s, which means it is a supersonic wave or shock wave. The wave tends to propagate faster along the wall due to the wall curvature effect. Both the color intensity and speed of the wave front tend to increase as it propagates, indicating the shock wave might be enhanced by the chemical reaction of the mixture behind the wave. In the other word, the wave is a supersonic reaction front. Note, we do not believe the reaction front is due to sequential autoignition of the unburned mixture because the reaction front is very smooth. Sequence autoignition, however, is usually more random and the reaction front is highly depending on the temperature gradient of the unburned mixture.

At the time of image L, two much brighter reaction fronts were formed at the right side of the combustion chamber. One propagates upward into the already partially burned mixture at a speed of 2086 m/s. The other propagates into the unburned mixture, whose light intensity is much brighter. The speed of the wave along Paths 3 and 4 (Figure 3b) are 2235 and 2608 m/s. Since the C-J detonation speed of the unburned mixture is about 1840 m/s, it is very clear that the reaction fronts are due to mixture detonation.



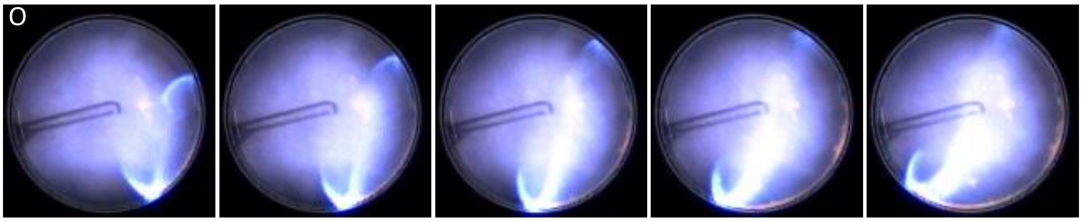
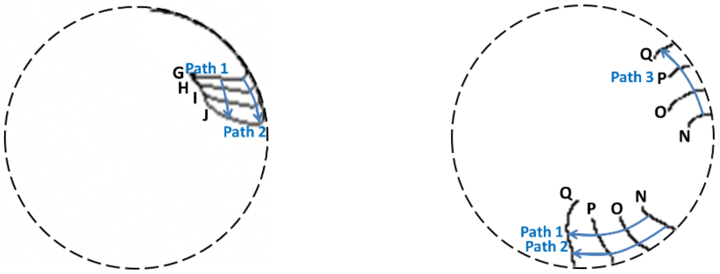
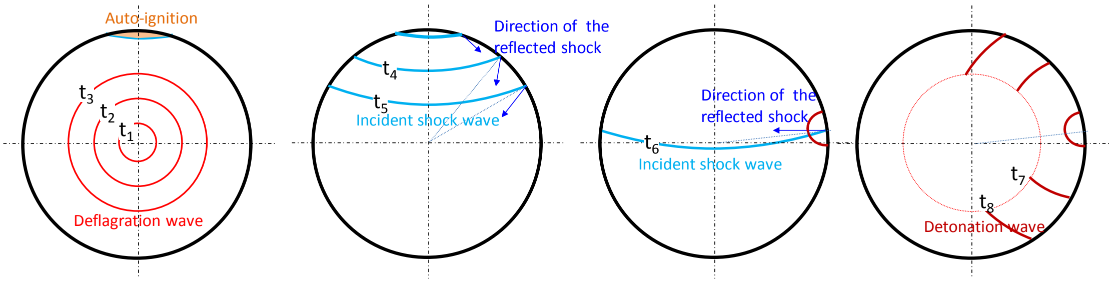


Figure 2. High speed images of SWRID (frame interval=3.47 μs, the intensity to the first ten images have been enhanced by 5 times with background noise subtracted)



(a) wave before detonation (b) detonation wave

Figure 3. Propagation paths of the shock wave before detonation and the detonation waves



a) Deflagration propagation b) Shock wave propagation c) Detonation initiation d) Detonation propagation

Figure 4. Illustration of the SWRID initiation process

The SWRID has the following features: (1) the end gas was compressed due to the heat release of the spark triggered turbulent flame propagation (Figure 4a); (2) A relatively strong local end gas auto-ignites, which causes local sudden pressure rise and generates a shock wave (called incident shock wave in Figure 4b) The incident shock wave propagates into the unburned mixture; (3) The incident shock wave is reflected by the cylinder wall. When the reflected shock wave does not interfere with the incident shock wave (shown in Figure 4b), it does not cause detonation; (4) When the incident shock wave propagates to the region that the reflected shock wave interferes with the incident shock wave (shown in Figure 4c), detonation is initiated and propagates in the unburned mixture (Figure 4d), which causes severe pressure oscillation in the combustion chamber.

It is easy to understand that the autoignition initiated shock wave elevates the unburned mixture pressure and temperature, causing faster mixture reaction. However, the ignition delay of the mixture behind the incident shock wave is still too long even under these elevated pressure and temperature condition. If the reflected shock wave interferes with the incident shock wave, it further elevates the mixture pressure and temperature and ignites the mixture instantaneously. The heat release of the mixture thus couples with the shock wave, resulting in detonation, which could propagate at a speed even faster than the C-J detonation speed. Based on the above analysis and confirmed by the high speed images, the detonation is typically initiated near the cylinder wall and about 90 degree to the autoignition location.

4 Conclusion

This study presents the most frequently observed detonation initiation mode (shock wave reflection induced detonation, SWRID) in stoichiometric iso-octane/air mixture under high temperature and high pressure conditions relevant to the boosted IC engines. The major conclusions are:

1. In high temperature and high pressure closed combustion chamber, the local mixture auto-ignition induces the shock wave.
2. The SWRID consists of four stages: (1) the end gas was compressed by spark triggered deflagration, (2) A local end gas auto-ignition generates a shock wave and the shock wave propagates into the unburned mixture, (3) The incident shock wave is reflected by the cylinder wall, (4) When the incident shock wave propagates to the region that the reflected shock wave interferes with the incident shock wave, detonation is initiated, which causes detonation propagation.
3. Before detonation was initiated, the speed of the combustion wave front was less than that of C-J detonation speed (around 1840 m/s). Once the detonation was initiated, the detonation speed can be much higher than that of the C-J detonation.

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