Shock Wave and Flame Front Induced Detonation in Rapid Compression Machine

Yingdi Wang[1], Shouzhi Xiang[1], Yunliang Qi[1], Rémy Mével[2,3] and Zhi Wang[1,2,3]
[1] State Key Laboratory of Automotive Safety and Energy, Tsinghua University, Beijing, China
[2] Center for Combustion Energy, Tsinghua University, Beijing, China
[3] Department of Automotive Engineering, Tsinghua University, Beijing, China

1 Introduction

One strategy to improve the efficiency of spark ignition internal combustion engine, SI-ICE, is to increase the power density through high boosting. However, under such conditions, super-knock can occur and constitutes the major obstacle for the development of the next generation of SI-ICE. Although it has been demonstrated using a rapid compression machine, RCM, that detonation can be initiated during this process [1], the initiation mechanism remains unclear. The mode of ignition in RCM is influenced by the in-homogeneity of the test volume induced by heat transfer and mixing [2]. Numerous studies have investigated the impact of reactivity gradient on the mode of propagation of combustion waves. In his pionnering analysis, Zeldovich [3] distinguished four modes of reaction: (1) "weak detonation"; (2) "normal detonation"; (3) subsonic flame unaffected by heat conductivity; (4) "normal flame". Bradley et al. [4] and Gu et al. [5] derived a detonation peninsula in the (ξ,ϵ) space from one-dimensional simulation performed under conditions representative of internal combustion engine at high loads, where ξ is the actual temperature gradient at the hot spot normalized by the critical gradient and ϵ is the ratio of acoustic time to the excitation time of local homogeneous mixture. More recently, Dai et al. [6, 7] studied reaction front propagation in n-heptane/air mixtures with a hot or cool spot using one-dimensional numerical simulations with with a skeletal kinetic model containing low temperature chemistry. They showed that both configurations could result in the initiation of a detonation wave. All these previous studies have employed one-dimensional numerical simulations and, despite providing important insight into the dynamics of end-gas auto-ignition and subsequent combustion wave propagation, they constitute an over-simplified description of the actual configuration.

The present study aims at clarifying the mechanism of detonation initiation under super-knock relevant conditions. Experimental work in a RCM and two-dimensional numerical simulations with skeletal chemistry are combined to unravel the dominant steps of detonation initiation under super-knock conditions in SI-ICE. In a previous study [8], the dynamics of one mode of initiation, namely shock wave reflection induced detonation (SWRID), has been revealed through high speed direct photography in RCM. The present paper focuses on another mode referred to as shock wave and flame front induced detonation (SWFID).

Correspondence to: qiyl@tsinghua.edu.cn

2 Experimental and computational methods

2.1 Rapid compression machine

DDT experiments were conducted in a rapid compression machine (RCM) at Tsinghua University. A detailed description of the experimental set-up and the data processing procedure can be found in Di et al. [9]. Briefly, the RCM has a fixed stroke of 500 mm and a combustion chamber diameter of 50.8 mm. The mixture in the test section was brought to high pressure and temperature within 30 ms. A creviced piston design was used to minimize the effect of the roll-up vortex. A piezoelectric pressure transducer (Kistler 6125C) and quartz window were mounted on the side and end wall of combustion chamber, respectively. The images were recorded using a high speed camera (Photron SA-Z) at frame rate 288,000 fps (frame interval of 3.47 μs). The spark plug (Denso K20R) was mounted at the opposite side of the pressure sensor with electrodes located at the center of the combustion chamber to generate a flame and was triggered at the end of compression, EOC. The schematic of the RCM is shown in Figure 1.

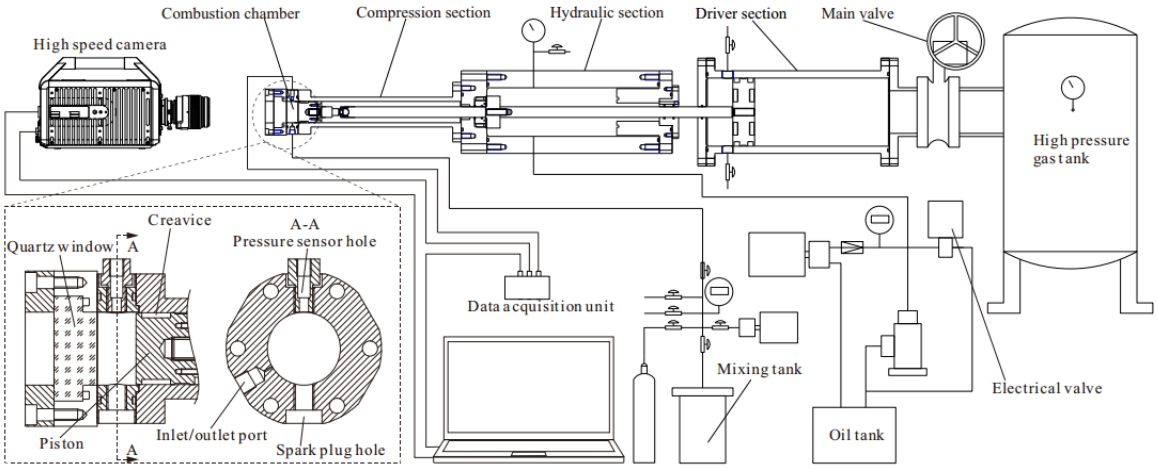


Figure 1: Schematic of the rapid compression machine [10].

2.2 Test Mixture

Stoichiometric iso-octane/air mixture was used, i.e. the molar ratio of iso-octane:oxygen:nitrogen was 1:12.5:47. The mixture was prepared using a dedicated stainless steel mixing tank at room temperature (302 K). The compression ratio in this study was 9.8 so that the temperature and pressure reached 641 K and 2.5 MPa at the EOC.

2.3 Computational method

The CONVERGE CFD code with AMR method [11] was used to simulate the detonation initiation process. Considering the compromise of detonation scale and computational cost, self-adaptive mesh with a basic grid size of 0.2 mm and a minimum of 25 μm was used. A renormalization group, RNG, k-ϵ turbulence

model was employed. Adiabatic non-slip bondary conditions were used at the wall. In terms of chemical kinetics model, a reduced primary reference fuel, PRF, model, referred to as GRON model [12] with 22 species and 21 reactions was used. The initial conditions were derived from experiments. The pressure was 7.46 MPa at the onset of auto-ignition. Assuming an isentropic compression of the fresh mixture during the propagation of the spherical flame, the temperature was calculated to be 820 K in the unburnt region. In the burnt region, the temperature was set at 2500 K. Because (i) the conditions at the wall are not relevant to the detonation onset at the expanding flame front and (ii) a structural hot spot was likely to exist to trigger auto-ignition in the experiment, a temperature of 1000 K was imposed at the top boundary in the computational study. This is shown in Figure 2. This hot wall enabled to create a realistic temperature gradient and to trigger the end gas auto-ignition.

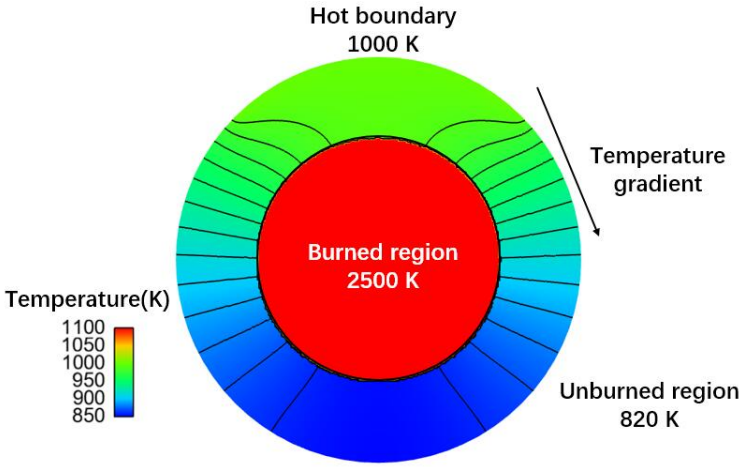


Figure 2: Schematic of the computational domain with initial and boundary conditions. The solid lines represent iso-contours of temperature.

3 Results and discussion

Figure 3 compares the experimental self-luminescence images and the numerical simulations of the SWFID process. The numerical images present the pressure and temperature distribution along with the HCO radical field, which represents the flame front or preheat zone, and the OH radical field which represents the reaction zone. The simulation reproduces the main features observed experimentally and demonstrates overall qualitative agreement. The combustion wave propagates downward from the strong local explosion at the top wall and interacts with the spherically expanding flame ignited by the spark plug. At t=377 μs, a curved reaction front as well as a zone of intense luminosity at the side wall can be observed on the left side of the experimental image. These two features are also seen in the two following images at t=380.5 and 384 μs. From the numerical simulations, it seems that the curved reaction front corresponds to a developed detonation wave which propagates both downward and toward the wall. The reflection of the detonation at the side wall creates the localized zone of intense luminosity which is seen in the simulation as a region of high pressure and high OH concentration. Extracting the propagation paths of the detonation wave from experimental results, the average speed is calculated as 1730 m/s (Ma=3.2) , which means a 6.3% deficit compared to the local Chapman-Jouguet velocity for the mixture (D_{CJ}=1847 m/s).

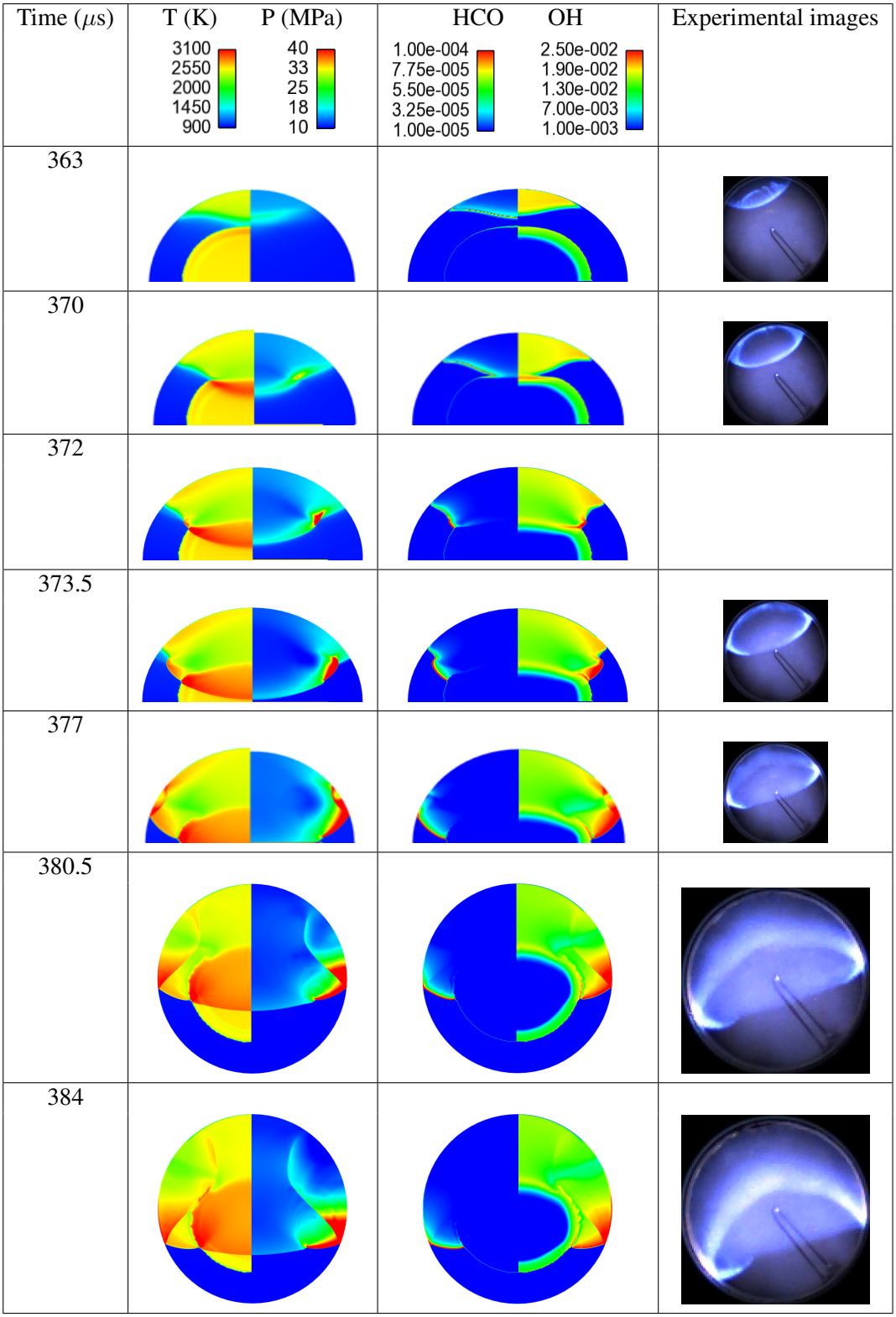
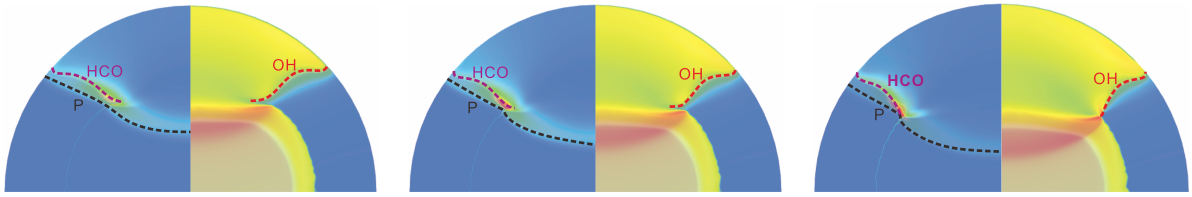


Figure 3: Numerical and experimental SWFID phenomenon.

To gain further insight into the mechanism of detonation initiation, temperature, pressure and species concentration fields at detonation onset were examined. These results are displayed in Figure 4. At t=369 μs, a region of higher pressure and temperature is created at the intersection of the shock fronts propagating in the burnt and in the unburnt gas region. The pressure at this location is the highest in the computational domain whereas the maximum temperature is located in the region of burnt gas compressed by the shock wave originating form the end gas ignition. Nevertheless, the temperature at the interception of the two shock fronts is several hundred kelvin above that of the fresh mixture compressed by the end-gas shock wave. This localized higher temperature enables the flame front to accelerate, t=370 μs, and catches up with the shock front, t=371 μs, to eventually form a self-sustained detonation wave. To summarize this mode of super-knock initiation through the SWFID process, the main steps are illustrated schematically in Figure 5.



t=369 μs t=370 μs t=371 μs

Figure 4: Superimposed pressure field and HCO front (left) and temperature field and OH front (right) at detonation onset. On the left, the front of the shock wave induced by the top wall explosion is also shown as black dashed lines.

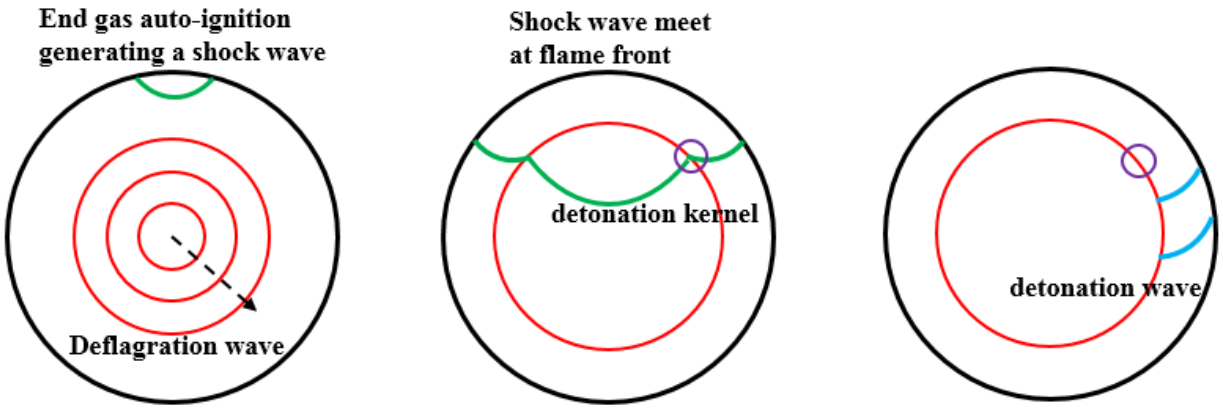


Figure 5: Main steps of the SWFID process.

4 Conclusion

A combination of experimental and numerical method was used to analyze the detonation initiation process of stoichiometric iso-octane/air mixtures in a RCM under engine relevant conditions. The mechanism of SWFID was revealed. This process can be divided into six steps:
1) Spark triggered spherical deflagration wave propagates and compresses the end gas

2) End gas auto-ignition produces a shock wave
3) Shock wave propagates into the burnt region and accelerates to catch up with the shock front propagating in the near wall unburnt region
4) Shock waves intersect at the front of the spherical flame which leads to a pressure and temperature rise
5) The flame front originating from the end gas auto-ignition accelerates due to the higher temperature in the region just ahead of it
6) The flame front couples with the shock wave which results in a self-sustained detonation

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