



# Pressure wave evolution during two hotspots autoignition within end-gas region under internal combustion engine-relevant conditions



Haiqiao Wei\*, Ceyuan Chen, Gequn Shu, Xingyu Liang, Lei Zhou

State Key Laboratory of Engines, Tianjin University, Tianjin 300072, PR China

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## ABSTRACT

To further understand the intense pressure wave formation mechanism induced by multiple spontaneous ignition kernels under internal combustion engine-relevant conditions, a one dimensional code to solve the Navier–Stokes equations for reactive flows is adopted in this parametric study. The multiple autoignition kernels occurring in the end-gas region are simplified into two neighboring hotspots. Stoichiometric mixtures of PRF40/air (without an obvious Negative Temperature Coefficient (NTC) behavior, and showing a certain degree of anti-knock property) and PRF0/air (exhibiting a strong NTC behavior and weak anti-knock property) are both used to explore the effect of fuel characteristic. The initial pressure is 30.0 atm. Unburnt gas temperatures of 800.0K and 890.0K are below and within the NTC regime of stoichiometric PRF0/air under the initial pressure. The hotspots are modeled as sine waves in the initial temperature field. Different sine wave amplitudes are adopted to examine the effect of temperature inhomogeneity. Within a limited computational domain, a detonation wave tends to form under the initial conditions with a small interval between hotspots, a low initial temperature of the unburnt mixture and a large temperature inhomogeneity. During the formation of detonation wave, a process similar to the “explosion in the explosion” phenomenon that are found in previous experiments has been detected. Moreover, at the low initial temperature, a large interval between hotspots reduces the maximum intensity of pressure wave. In contrast, a wide interval increases the maximum pressure intensity at a higher initial temperature. The strongest pressure intensity induced by PRF0/air mixture autoignition is generally higher than that during the autoignition of PRF40/air mixture under the same initial condition, but a common intense pressure wave generation mechanism is shared. Furthermore, compared with the autoignition of the PRF40/air mixture, the distance for detonation formation within PRF0/air mixture becomes shorter.

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## 1. Introduction

Downsizing technology combined with turbocharging has been proven as a practical method for improving the efficiency of spark ignition (SI) engines. However, the gas-phase autoignition propensity increases with a higher downsizing level. Intense pressure waves or even detonation waves that form within the reactive end gas can lead to abnormal combustion phenomena, e.g., knocking combustion and low speed pre-ignition (LSPI) which are characterized by a strong pressure oscillation [1]. Also, spark-assisted compression ignition (SACI) combustion are similar to SI engine knock in that the end gas autoignition occurs before being completely consumed by a turbulent flame [2]. Relevant phenomena induced by combustion instability are also reported in other combustion devices [3–4]. The main differences in combustion characteristics

between gas turbine engines, rocket engines and internal combustion (IC) engines are the thermochemical state of unburnt mixture. In addition, the combustion of IC engines occurs in a time-varying enclosure space.

IC engines combustion anomalies are stochastic and can cause mechanical structure damage to research engines, therefore, numerical studies have become attractive for engine combustion researches. It has been widely accepted that the occurrence of autoignition is a necessary but not sufficient condition for abnormal combustion. The pioneering work of Zel'dovich [5] classified the modes of the propagation combustion waves that originate from an autoignition kernel surrounded by a non-uniform distribution of chemical reactivity. Gu et al. [6], Bradley and Kalghatgi [7] and Bates and Bradley [8] quantified different propagation modes on a diagram of  $\xi$ – $\varepsilon$  coordinates, where  $\xi$  is the acoustic speed normalized by the autoignition flame velocity, and  $\varepsilon$  represents the acoustic wave residence time in the autoignition kernel. Five reaction front propagation modes, namely, thermal explosion, supersonic auto-ignitive deflagration, developing and developed

\* Corresponding author.

E-mail address: [whq@tju.edu.cn](mailto:whq@tju.edu.cn) (H. Wei).

detonation, subsonic auto-ignitive deflagration, and normal flame deflagration, have been clearly identified. Wang et al. [9] employed a 1-D computational fluid dynamics (CFD) simulation to explore the autoignition and pressure wave development during the LSPI. The 1-D simulations of Dai et al. [10] validated the applicability of Zel'dovich's theory [5] to engine knock by considering the negative temperature coefficient (NTC) behavior of *n*-heptane. Further investigation of Terashima and Koshi [11] compared the pressure wave generation process for *n*-butane/air and *n*-heptane/air mixtures using a 1-D constant volume reactor. The results showed that the NTC behavior influences the timing of the pressure oscillation. Moreover, by considering the interaction of the autoignition flames and pressure waves reflected on the wall, their work revealed that the size and position of autoignition kernels relative to the cylinder wall had a significant effect on the pressure oscillation intensity. In addition, examining the effect of turbulence on the autoignition regime is important to achieve a comprehensive understanding of abnormal combustion phenomena. The turbulence-chemistry interaction mechanism has been studied in Refs. [12–14].

Furthermore, it has been noted that the autoignition inside a cylinder is always characterized by multiple kernels that are randomly located within the end-gas region [15,16]. In practice, a slight temperature non-homogeneity inside a cylinder, induced by gas exchange or heat transfer, is sufficient to provoke several autoignition kernels [17]. This is expected to result in the mixed modes of autoignition. Robert et al. [18] explored different scenarios for knock and super knock in SI engines. The results showed that the highest pressure oscillation intensity corresponded to the case of which a pressure wave coupled with several local autoignition spots. Hence, the multiple-kernel autoignition process should be analyzed to further explore the mechanism of abnormal combustion phenomena. The simulation results of multiple kernels could be too noisy to analyze the physical and chemical processes, therefore, the pioneering studies generally adopt the simplification achieved with two hot spots. Pan and Sheppard [19] used a two-dimensional CFD code to study the effect of the relative positions and autoignition sequence (sequential autoignition or simultaneous autoignition) of two kernels within a stoichiometric iso-octane/air mixture. In their study, the distance between hot spots was much larger than the scale of hotspots. It was found that, in sequential autoignition spots case, pressure waves emanating from the first spot could modify the temperature gradient near the second spot and thereby, changed the autoignition mode. However, the detailed formation process of a strong pressure pulse or detonation induced by the interaction between pressure waves and reaction waves is difficult to capture. Hajireza et al. [20] adopted a detailed chemical mechanism of primary reference fuel (PRF), a bi-component mixture of *n*-heptane and iso-octane, to explore the low- and high-temperature reactions during two spots autoignition process as a function of the degree of temperature homogeneity. In their study, different reaction front velocities, ranging from several meters per second to 55 m/s, propagating from the exothermic kernel were observed. However, as the pressure was assumed to be homogeneously distributed, the pressure wave propagation could not be detected. It is worth noting that 1-D numerical study generally adopts some simplifications. However, it is able to offer some important qualitative results through isolating the concerned factor. In the present study, the pressure wave evolution during two hotspots autoignition is simulated by a parallelized version of a 1-D unsteady reactive flow (A-SURF) code [21]. A high performance implementation of the Message Passing Interface (MPI), MPICH [22, 23] is adopted. The computational domain is the end gas region, effects of turbulence and the compression of end gas induced by the propagation of main flame (triggered by the spark plug) are not considered here. To analyze the effect of fuel characteristic on the pressure wave evolution, two fuel surrogates, i.e., PRF40 (40%

iso-octane and 60% *n*-heptane by volume) and PRF0 (0% iso-octane and 100% *n*-heptane by volume) are selected. PRF40 exhibits a weak NTC behavior and has a certain degree of anti-knock property, while PRF0 shows a strong NTC behavior and a knocking tendency. The chemical characteristics of other PRFs with iso-octane volumetric fraction less than 40%, such as PRF10 or PRF20, fall someplace between them, so are the behaviors during autoignition process. Furthermore, the ignition delay times of the stoichiometric PRF40/air and PRF0/air mixtures obtained under a typical pressure at top dead center (30.0 atm) are close to the combustion duration of the IC engines. PRFs with volumetric fraction of iso-octane above 40% show a weak NTC behavior which are similar to PRF40, but the ignition delay times could increase by an order of magnitude. Thus, the mechanism of strong pressure wave generation during end gas autoignition can be explored with an affordable and reasonable simulation time (close to the engine-relevant conditions) through using PRF40 and PRF0. Moreover, some previous studies also employed PRF40 and PRF0 as surrogate fuels for end gas autoignition of IC engine. Hajireza et al. [20] explored the hot-spot autoignition in SI engines through considering PRF40 as the surrogated fuel, and some critical phenomenon of SI engines can be addressed. Wei et al. [24] studied the autoignition of PRF0/air mixture in the end-gas region, and the two-stage ignition process i.e. low- and high-temperature chemistries have been considered. Ju et al. [2] have considered *n*-heptane as the fuel of SACI. It should be noted that a commercial IC engine fuel is a complex mixture of hundreds of hydrocarbons, and the PRFs cannot fully emulate the chemical kinetic characteristic of real fuels, which are knock rated [25]. However, the PRFs can provide us valuable insight regarding the combustion behavior of hydrocarbons/air mixtures under engine-relevant conditions.

The outline of the remainder of this paper is as follows. The numerical method and simulation conditions are introduced in Sections 2 and 3. The analysis of the parametric study is discussed in Section 4. The conclusions are presented in Section 5.

## 2. Numerical method

To simulate the 1-D combustion process by solving the Navier-Stokes equation for multi-species reactive flows, a new parallel version of the A-SURF is adopted. The conservation equations of the reactive compressible flows are [26]

$$\partial U / \partial t + \partial F(U) / \partial x = \partial F_v(U) / \partial x + S_R, \quad (1)$$

where  $U$ ,  $F(U)$ ,  $F_v(U)$  and  $S_R$  are defined as follows:

$$U = \begin{pmatrix} \rho Y_1 \\ \rho Y_2 \\ \vdots \\ \rho Y_n \\ \rho u \\ e \end{pmatrix}, F(U) = \begin{pmatrix} \rho u Y_1 \\ \rho u Y_2 \\ \vdots \\ \rho u Y_n \\ \rho u^2 + P \\ (e + P)u \end{pmatrix}, F_v(U) = \begin{pmatrix} -\rho Y_1 V'_1 \\ -\rho Y_2 V'_2 \\ \vdots \\ -\rho Y_n V'_n \\ \tau \\ q \end{pmatrix}, S_R = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \vdots \\ \omega_n \\ 0 \\ 0 \end{pmatrix}. \quad (2)$$

Above,  $P$  is the pressure,  $\rho$  is the density,  $u$  is the velocity, and  $e$  is the total energy per unit mass.  $Y_k$ ,  $V'_k$ , and  $\omega_k$  are, respectively, the mass fraction, diffusion velocity, and production rate of species  $k$ .  $n$  is the number of species considered.

Eq. (1) is discretized by the finite volume method. Through utilization of the second-order splitting fractional-step procedure, the evolution of the stiff reaction term is separated from that of the convection and diffusion terms. The reaction source term is solved in the second fractional step by using the VODE solver, and the chemical kinetic calculations are conducted by the CHEMKIN [27] package. The mixture's average thermal and transport properties are evaluated by the TRANSPORT [28] package. To calculate the

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