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End-gas autoignition and detonation development in a closed chamber

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ABSTRACT

It is generally accepted that knock in spark ignition engines might be caused by end-gas autoignition. However, the detailed mechanism for autoignition-induced pressure oscillation and detonation development is still not well understood. This work studied end-gas autoignition and detonation development in a closed chamber using 1D simulation. Stoichiometric hydrogen/air mixture at different initial temperatures and pressures was considered and detailed chemistry was included in simulation. The objectives were to identify possible modes of end-gas combustion and to understand the mechanism of autoignition-induced pressure wave and detonation development. Depending on the chamber length as well as the initial temperature and pressure, there are three modes of end-gas combustion: normal flame propagation without autoignition, autoignition without detonation development, and detonation development. The amplitude of pressure oscillation was found to be determined by the mode of end-gas autoignition: autoignition can induce high amplitude of pressure oscillation similar to conventional knock; and detonation development can cause extremely high amplitude of pressure oscillation similar to super-knock. It was shown that autoignition and detonation development can be induced by increasing the initial temperature, initial pressure, or chamber length. The evolution of states of different flow particles was tracked and the combustion mode was found to switch from constant-pressure to constant-volume when autoignition occurs. The coupling between pressure wave and chemical reaction was analyzed and the mechanism for autoignition front acceleration and detonation development was investigated. Moreover, autoignition in end-gas with different values of ignition progress was simulated. It was demonstrated that high reactivity of end-gas promotes autoignition and detonation development.

1. Introduction

Downsized and boosted direct injection spark ignition engines (SIE) have the advantages of higher thermal efficiency and higher power density compared to traditional gasoline engine with large displacement. Therefore, it can be used to reduce fuel consumption. However, in highly-boosted gasoline engines, there is stronger tendency of knock when the premixture is compressed to higher temperature and pressure [1–4]. When knock occurs, high-frequency pressure oscillation can cause severe engine damage.

It is generally accepted that knock in spark ignition engines is caused by end-gas autoignition [5–7]. When premixed flame propagates in a closed chamber, the unburned gas (end-gas) is progressively compressed and its temperature and pressure continuously increase. Under appropriate conditions, autoignition occurs in end-gas before the propagating flame can consume the fuel. Heat release during local autoignition generates pressure pulse/wave which propagates across the system. The unburned mixture immediately behind the pressure wave might be compressed to react rapidly and, in turn, further enhance the pressure wave [4, 5, 7]. A detonation develops if there is a coherent coupling between pressure wave and local reaction/autoignition [8, 9]. The pressure wave propagates back-and-forth inside the closed chamber since it is reflected on the boundary walls. Consequently, high-frequency pressure oscillation or knock occurs.

In the literature, there are extensive studies on end-gas autoignition since it is closely related to engine knock. Theoretically, Strickland-Constable [59] and Livengood and Wu [10] studied flame propagation in an auto-ignitive mixture and proposed an integral method to predict the occurrence of autoignition; Zel'dovich [8, 11] first analyzed different modes of reaction front propagation caused by autoignition in a mixture with non-uniform reactivity; Bradley and coworkers [3, 6, 12–15] further investigated autoignition from a hot spot and proposed an operational peninsula in the plot of two non-dimensional parameters, namely the normalized temperature gradient and the ratio of acoustic time to excitation time (the operational peninsula can be used to determine the critical conditions for detonation development); Kagan and Sivashinsky [16, 17] analyzed end-gas autoignition in a one-dimensional (1D) closed chamber and proposed a 0D model to predict autoignition. However, one-step global

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reaction was usually assumed in theoretical analysis. Since complicated chemical kinetics is involved in ignition process, detailed chemistry needs to be considered for end-gas autoignition.

Experimentally, high speed photograph technology was used to visualize end-gas autoignition in engine (e.g., [2, 18, 19]) and rapid compression machine (RCM) [4, 20, 21]. Inside the engine and RCM, the flame front and flow are three-dimensional and thereby it is difficult to understand the interaction between pressure wave and chemical reaction during the autoignition process. To overcome this difficulty, Nagano et al. [22] and Qi et al. [23] designed quasi 1D experiment using a closed tube-shaped vessel to study end-gas autoignition and pressure oscillation. In these experiments, end-gas autoignition was successfully observed. However, the process is not truly 1D since there is strong flame-boundary layer interaction during flame propagation in a tube. Consequently, such experiments still have limitations in terms of understanding autoignition and pressure wave-chemistry interaction. (The truly 1D experiment for end-gas autoignition is to use a spherical bomb: first the premixture is preheated to high-enough temperature; then the mixture is centrally ignited which results in an outwardly propagating spherical flame; finally autoignition occurs in the unburned mixture after it is compressed by the outwardly propagating spherical flame. However, the spherical bomb might be damaged by strong pressure oscillation or detonation induced by end-gas autoignition.)

Numerically, multi-dimensional simulations were conducted to investigate the end-gas autoignition process. For examples, Pan et al. [24, 25] conducted 2D simulations to identify distinct autoignition modes and their contribution to knock; Liberman et al. [26, 27] conducted 2D and 3D simulations to examine the onset of autoignition; Wang et al. [28] conducted 3D simulations to study the coupling between pressure wave and chemical reaction; Wei et al. [29] conducted 2D simulations to assess the effects of pressure wave on end-gas autoignition; and Chen, Yoo and coworkers conducted 2D simulations to assess the effects of turbulence on autoignition (e.g., [30–33]). Similar to experiments, the autoignition process is very complicated in multi-dimensional simulations. Moreover, complicated chemistry involved in autoignition is difficult to be included in multi-dimensional simulations. Therefore, 1D simulations were used to study the autoignition process: Ju et al. [34] identified different flame regimes of ignition in n-heptane/air mixtures; Martz et al. [35, 36] demonstrated that the autoignition process is chemically controlled and diffusion can be neglected; Zhang [37] examined the effects of thermal stratification on autoignition within the negative-temperature coefficient (NTC) regime; Dai et al. [38] demonstrated that different autoignition modes can be initialized from a cool spot when the initial temperature is in the NTC regime; and Terashima and Koshi [39] investigated the strong pressure wave generated by end-gas autoignition. However, unlike the present study, detonation development caused by end-gas autoignition was not identified in these 1D studies except our recent work [38].

This work studied end-gas autoignition and detonation development in a closed chamber using 1D simulation with detailed chemistry. The interaction between pressure wave and chemical reaction was investigated. The objectives were to identify possible modes of end-gas combustion and to understand the mechanism of autoignition-induced pressure wave and detonation development. While multidimensional simulations describe the end-gas autoignition process similar to that occurs in practice, it is difficult to explain the detailed structure (evolution of the distributions of temperature, pressure and species concentrations) of autoignition and detonation development processes which might be complicated by turbulent flow and flame-boundary layer interaction. A 1D simulation was conducted here since detailed structure of autoignition and detonation development can be readily obtained and the pressure wave-chemistry interaction can be isolated from turbulent flow and flame-boundary layer interaction.

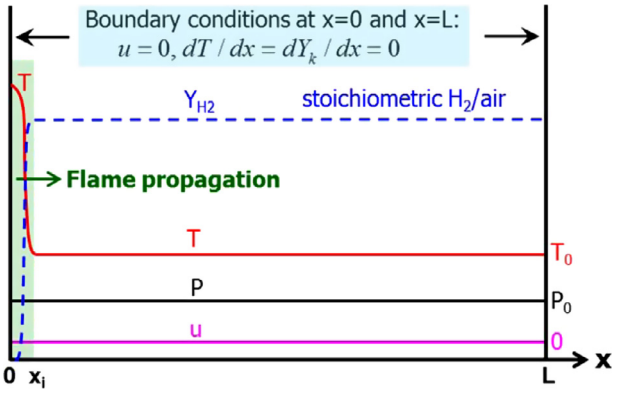

Fig. 1. The initial and boundary conditions used in the simulation of flame propagation in a 1D closed chamber with the length of L.

It should be emphasized that the in the present work we used 1D simulations to study the interaction between pressure wave and chemical reaction and the mechanism of detonation development, which are related to knock in engines. However, engine knock cannot be fully represented by simulations in the present work since our 1D simulations have the following limitations: (1) 3D effects including turbulence, boundary layer and wall heat transfer (which play major roles in engine knock) were not considered in the present 1D computation; (2) temperature inhomogeneity (local hot-spot) occurring in practical engines was not taken into account and the initial temperature of end-gas was assumed to be uniformly distributed; and (3) the fuel, initial temperature and pressure, domain dimension considered in the present study were not prototypic of an engine.

2. Model and numerical methods

2.1. Model

We conducted 1D simulation for stoichiometric hydrogen/air mixture since the chemical mechanism for hydrogen oxidation is relatively well established and it has relatively small size. In the model, the premixed H_2/air flame propagates toward the right side in a 1D closed chamber; and the end-gas between the propagating flame front and the right wall is continuously compressed and thereby autoignition and detonation might occur in the end-gas.

The computational domain is $0 \le x \le L$, where L is the chamber length. The initial and boundary conditions are presented in Fig. 1. The initial temperature and pressure of end-gas are shown to be T_0 and P_0, respectively. The propagating flame was initialized by a hot kernel close to the left boundary (i.e., $0 \le x \le x_i \approx 0.5$ mm). The initial distributions for temperature and mass fraction of all species were from PREMIX [40] results for stoichiometric H_2/air at T_0 and P_0. In PREMIX [40], finite-rate chemical kinetic model and multicomponent molecular transport model were considered for a freely-propagating, adiabatic, planar flame. As shown in Fig. 1, initially the flow speed is zero (i.e., $u = 0$) everywhere and the initial pressure of P_0 is uniformly distributed in $0 \le x \le L$. The initial temperature of T_0 is uniformly distributed outside of the hot kernel (i.e., $x_i \le x \le L$). At both boundaries (i.e., $x = 0$ and $x = L$), zero flow speed and zero gradients of temperature and mass fractions are enforced.

2.2. Numerical methods

The transient flame propagation and autoignition process was simulated using the in-house code A-SURF [38, 41, 42]. The finite volume method was used in A-SURF to solve the conservation equations for 1D compressible flow with multi-components. The time evolution of the stiff reaction term was separated from that of the

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