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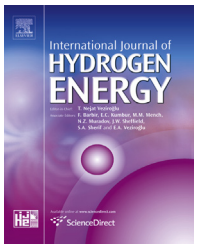

Interaction of pressure wave and propagating flame during knock

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ABSTRACT

To determine the mechanism of interaction between a pressure wave and a propagating flame during knock, normal combustion and knock are numerically modeled in a simplified one-dimensional hydrogen-fueled spark ignition engine. The heat release rate of the flame front during knock abruptly increases when the pressure wave propagates through the reaction zone. The pressure wave in the diffusion zone perturbs temperature and thus causes thermal runaway at positions with low temperature and high reactant concentrations. Analysis of the Damköhler number (the ratio of gas dynamic time to chemical reaction time) and the estimated overpressure revealed that abruptly raised heat release rate during knock facilitates the amplification of the pressure wave and reinforces the interaction between pressure wave and chemical heat release.

1. Introduction

Increasing the compression ratio increases the overall efficiency of spark ignition (SI) engines. However, a high compression ratio facilitates the occurrence of unburned end-gas auto-ignition, which is the onset of knock. Knock significantly accelerates local pressure, decreases thermal efficiency, and even destroys the cylinder. Given the complexity of its chemical and physical processes, the evolution and mechanism of knock remain inadequately explained. However, using detailed chemistry numerical simulation, which can provide highly detailed and abundant information about knock process, is a potential way to investigate the evolution and mechanism of knock.

For the studies of knock, numerical simulation methods can be divided into two types. One type is based on zero-dimension combustion models using a detailed chemical mechanism, such as models by Gogan and Sundén (with detailed chemistry) [1], Noda and Kazuya (with a semi-detailed chemical mechanism) [2], and Liu and Chen (with modified Tanaka's reduced chemical kinetic model) [3]. With regard to the evolution of knock, especially after end-gas auto-

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ignition, the interaction between the pressure wave and propagating flames in the cylinder most significantly affects the sustenance of knock. However, the zero-dimension model cannot provide any spatial information on knock evolution and on the interaction between the pressure wave and the flame.

The other type of numerical simulation methods is based on CFD (Computational Fluid Dynamics) modeling. The complex configuration like real cylinder is usually considered in such simulation. Several studies of this type are coupled with detailed chemistry [4,5], whereas most are coupled with highly reduced multi-step or single-step chemistry to avoid very large calculations [6–9]. For CFD-based numerical simulation in such configurations, the complexity of propagating flames and wave structures makes the knocking mechanism difficult to understand though the violent pressure oscillation in cylinder is obtained. Furthermore, those using simple chemistry prevent the simulation from reflecting the realistic chemical reaction effects on the evolution of knock. Therefore, due to the above intrinsic limitations, numerical studies in complex configuration still cannot fully reveal the knocking mechanism.

For the interaction between pressure wave and propagating flames which is fundamental process in knock formation and evolution, some theoretical and numerical studies [10–23] have investigated in highly simplified configurations. These studies have found important mechanisms that amplify pressure waves by auto-ignition, ranging from research on single auto-ignition centers [17,18] to that on propagating auto-ignitive reaction fronts [19–22]. The magnitude of amplified pressure waves depends on the ratio of the acoustic timescale to the excitation time for the single auto-ignition center and on the ratio of the acoustic timescale to the propagating timescale of the auto-ignitive reaction front for the successive auto-ignition mode. However, these highly simplified physical models without wall effects cannot reflect important realistic conditions for studying engine knock. Thus, we study the interaction between pressure waves and flame propagation by coupling CFD with detailed chemistry in a confined space. The most important factors for knock, such as the reflection and superposition of pressure waves, the coexistence of propagating multi-flame fronts as well as the variation of total pressure and temperature with time, are therefore considered in present study.

2. Physical model and numerical methods

The key factors for knock phenomena are SI-induced central propagating flames, walls that enable the propagation of acoustic waves in the cylinder, and end-gas auto-ignition. Based on these key factors, a simplified physical model for the knock phenomenon is proposed (Fig. 1). This model includes the initial introduced central flames, rigid walls at both ends of the computational domain, and a high-temperature, high-pressure artificial auto-ignition zone adjacent to the left wall. In this model, the propagating flame, pressure oscillation, and interaction between the flame and pressure wave are numerically simulated.

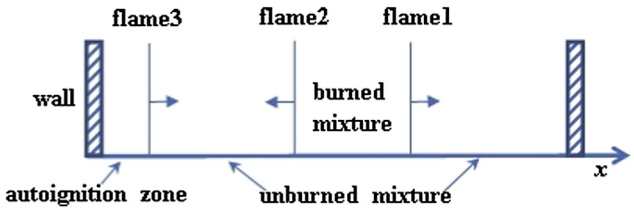

Fig. 1 – Schematic showing the physical model of knock in one-dimensional SI-engine reactor.

The knock phenomenon occurs in hydrogen-fueled internal combustion engines [24,25]. The oxidation mechanism of hydrogen is the simplest and most well developed. Therefore, we use hydrogen as the fuel in the numerical simulation. The central flames and auto-ignition zone with high temperature and pressure are set as initial conditions.

This study uses the stoichiometric mixture of hydrogen and air, an initial temperature of 750 K, and an initial pressure of 25 atm. Under these conditions, the detailed premixed planar flame structure is computed with the CHEMKIN PREMIX code [26] and then introduced to the center of the computational domain as the initial spark-ignited flame. Modeling knock assumes the occurrence of end-gas auto-ignition at the very beginning. Thus, a 1 mm-thick artificial auto-ignition zone of 2200 K and 50 atm is initially created. The total length of the computational domain is 5 cm. The homogeneous distribution of temperature and concentration of unburned gas is considered.

Based on this physical model, the one-dimensional unsteady compressible reactive flow is numerically solved using the in-house code A-SURF (Adaptive Simulation of Unsteady Reacting Flow) [27–29]. The following equations for a multi-species reactive mixture in a one-dimensional coordinate are solved in A-SURF:

$$\frac{\partial U}{\partial t}+\frac{\partial F(U)}{\partial x}=\frac{\partial F_v(U)}{\partial x}+S_R \tag{1}$$

where the vectors U, $F(U)$, $F_v(U)$, and S_R are defined as

$$U=\begin{pmatrix}\rho Y_1\\ \rho Y_2\\ \vdots\\ \rho Y_n\\ \rho u\\ E\end{pmatrix},\quad F(U)=\begin{pmatrix}\rho u Y_1\\ \rho u Y_2\\ \vdots\\ \rho u Y_n\\ \rho u^2+P\\ (E+P)u\end{pmatrix},\quad F_v(U)=\begin{pmatrix}-\rho Y_1 V_1'\\ -\rho Y_2 V_2'\\ \vdots\\ -\rho Y_n V_n'\\ \tau\\ q\end{pmatrix},$$
$$S_R=\begin{pmatrix}\omega_1\\ \omega_2\\ \vdots\\ \omega_n\\ 0\\ 0\end{pmatrix} \tag{2}$$

Here ρ is the density, u the flow velocity, and E the total energy per unit mass. The quantities, Y_k, V'_k and ω_k, are the mass fraction, diffusion velocity and production rate of species k, respectively. The production rates are specified via collection of elementary reactions using a CHEMKIN compatible database [26]. Similar to our previous study [30],