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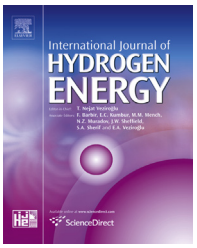

A numerical study on pressure wave-induced end gas auto-ignition near top dead center of a downsized spark ignition engine

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ABSTRACT

Auto-ignition of end gas is known as a main cause of knock in SI engine. In order to study the characters of auto-ignition induced by pressure wave, different levels of hot zones characterized by temperature gradients are created in end gas, which are then ignited by incident pressure wave developed from main flame. Evolutions of pressure and temperature in end gas are monitored to investigate pressure incidence and end gas auto-ignition. Computational Fluid Dynamics (CFD) calculations are carried out in a simplified two-dimensional symmetrical computational domain. Turbulence is modeled by renormalization-group (RNG) $k-\varepsilon$ model and the turbulence-chemistry interaction is modeled using Eddy Dissipation Concept (EDC) with a detailed chemical kinetic mechanism for hydrogen oxidation. Ignition delay sensitivity analysis is also employed to investigate chemical kinetics during the incidence of pressure wave. The results show that the incidence of pressure wave has significantly different effects on auto-ignition characteristics, thus resulting in different ignition delays, pressure oscillations and enhancements of reflected pressure wave.

Introduction

Downsized spark ignition (SI) engine plays an important role in energy conservation and emission reduction due to its high thermal efficiency resulted from the utilization of smaller cylinder volume and inlet air supercharging [1]. However, the supercharging level is limited by engine knock, in which situation pressure oscillation occurs and thermal efficiency decreases greatly. In severer situations, the engine suffers physical damage and heat erosion. Auto-ignition of hot spots with higher reactivity in unburned gas is considered as the main cause of engine knock [2]. Hot spots can be produced through quite complicated ways such as gas convection, heat transferred from hot surfaces and compression effect of pressure waves, all of which makes it stochastic for auto-ignitions to appear. Experiments [3,4] showed that the pressure profiles measured at different locations differ from each other during same knocking cycle, which indicates the existence of propagation, interaction and reflection of pressure waves inside combustion chamber. So it's an important issue to figure out how pressure wave is formed, how it initiates auto-ignition and what kind of knock it causes.

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When combustion proceeds, heat generated from flame front will raise local temperature thus driving hot gas compressing cooler surroundings. A pressure wave is then initiated and, if energy is sustainably gained from flame front, will gradually develop into a shock wave. Considering a zero-thickness normal shock propagating in one-dimensional flow, by solving conservation equations of mass, momentum and energy, relations between flow variables upstream and downstream can be expressed as follows:

$$\frac{p_1}{p_0} = \frac{2\gamma M_0^2 - \gamma + 1}{\gamma + 1} \tag{1}$$

$$\frac{T_1}{T_0} = \frac{(2\gamma M_0^2 - \gamma + 1)\left[(\gamma - 1)M_0^2 + 2\right]}{(\gamma + 1)^2 M_0^2} \tag{2}$$

$$\frac{\rho_1}{\rho_0} = \frac{(\gamma + 1)M_0^2}{(\gamma - 1)M_0^2 + 2} \tag{3}$$

where p, T, ρ, γ and M are the pressure, temperature, density and Mach number respectively. Subscript 0 and 1 indicate states upstream and downstream. For a pressure wave traveling at sound speed, $M_0 = 1$, therefore flow characters change continuously after pressure wave. However, pressure waves with high peak value will still make local temperature increase significantly when it propagates through unburned mixture or is reflected by the wall, thus making it faster for end gas to auto-ignite, even before the spark-ignited flame front arrives.

Large amount of researches focused on the initialization of flame front and pressure wave. The different regimes of flame front initialized by non-uniform initial conditions were first studied by Zeldovich using a one-step chemical model [5]. He figured out that spontaneous reaction wave can propagate through a reactive material along a spatial gradient of variables such as temperature and species concentration that could influence ignition delay. Considering an area with temperature gradient along x-axis, auto-ignition will first occur at the location where there has the highest temperature $T(x)_{max}$, the spontaneous reaction wave then propagates along the gradient with the speed u_{sp}:

$$u_{sp} = \left(\frac{\partial \tau_{ig}}{\partial x}\right)^{-1} = \left(\frac{\partial \tau_{ig}}{\partial T}\frac{\partial T}{\partial x}\right)^{-1} \tag{4}$$

where τ_{ig} is ignition delay as a function of initial temperature gained from experiment or chemical kinetics calculation. According to their relationships with Chapman–Jouguet speed and sound speed, different u_{sp} indicate the initializations of different regimes of spontaneous reaction wave, such as detonation, deflagration and homogenous explosion. The concept was afterwards studied computationally by Gu et al. [6] and Liberman et al. [7] with detailed chemistry that can properly reflects detailed development process of auto-ignition. Pressure wave-flame interaction in multi-dimensional models was also studied through CFD modeling. Khokhlov et al. [8–10] numerically studied shock-flame interactions in reactive mixture. They found that flame generates and enhances the shock waves, which in turn creates turbulence in flames thus promoting the formation of hot spots, causing auto-ignition and Deflagration-to-Detonation Transition (DDT). Similar effects of pressure wave on flame were also observed by Molkov et al. [11]. They modeled hydrogen-air deflagration in a long tunnel, where initial pressure wave develops into a shock due to reflection by obstacles. As engine knock is characterized by strong pressure oscillation in cylinder, numerical researches were also carried out to investigate its relations with pressure wave and chemical reactions. Zhi Wang et al. [12] modeled an SI engine using RNG $k-\varepsilon$ turbulent model and G-equation combustion model coupled with detailed Primary Reference Fuel (PRF) mechanism. It was found that interaction of pressure wave and chemical reactions occurs near the wall during knock, thus leading to a high frequency pressure oscillation in the high temperature gas near wall.

Despite large amount of works that have been done, there's still a lack of investigations on interaction between pressure wave and auto-ignition under engine-relevant conditions. The objective of this paper is to illustrate how auto-ignition is induced by pressure wave, the effects that auto-ignition may have on pressure waves and how it will influence engine knock. Numerical simulations are carried out in a two-dimensional computational domain, which has the same scale as the combustion chamber near Top Dead Center (TDC). At first fuel is ignited by a high temperature zone. As flame front is formed with a pressure wave propagating away from flame front, different levels of end gas non-uniformities characterized by linear temperature gradients are introduced in end gas to initialize auto-ignition of different intensities and ignition delay. Zero-dimensional homogenous ignition delay tests are also implemented to analyze the chemical kinetic details during pressure wave induction.

Numerical details

Grids details and physical model

The key issue in this simulation is to correctly capture the characters of the pressure wave especially when discontinuity appears, and to ensure both the stability and accuracy of calculation when flow-chemistry is strongly coupled. So it's of great importance to verify if the observed characters of pressure wave are correctly resolved. Mesh size usually depends on the size of whole computational domain and the characters of the problem to be solved, whose scales range from micrometer to meter [7,11]. Study on mesh convergence is performed within several empirical cell sizes, at last a cell size of 0.1 mm × 0.1 mm is chosen in consideration of both the ability to capture flow discontinuity and the reduction of computational cost. Fig. 1 shows the schematic of mesh information and detailed setup of the computational domain. 29,133 cells are generated in a two-dimensional symmetrical computational domain with a size of 4 mm × 75 mm, which accounts for half of a combustion chamber at TDC. A two-dimensional domain is selected to reflect the complex flow caused by pressure wave in finite space while limiting computational cost to a lower level. Mesh is refined to half its size near wall to increase calculation accuracy considering pressure wave reflection and end gas auto-ignition. Static grids instead of dynamic grids are selected for better ability to