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One-dimensional numerical study on pressure wave–flame interaction and flame acceleration under engine-relevant conditions

Haiqiao Wei*, Yibao Shang, Ceyuan Chen, Dongzhi Gao, Dengquan Feng

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

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ABSTRACT

Knock is considered as a major challenge when increasing thermal efficiency of internal combustion engine. In this study, two possible causes of engine knock: flame acceleration and auto-ignition, are studied using one-dimensional simulation under engine-relevant conditions. Chemical source term is modeled using Arrhenius expression with detailed chemical mechanism of hydrogen oxidation. Interaction between pressure wave and flame during propagation of flame front is investigated. It is observed that propagation and reflection of pressure wave in cylinder might trigger Deflagration–Detonation Transition (DDT), which leads to extremely high pressure oscillation. Pressure wave initialized by auto-ignition flame is also a reason leading to detonation by enhancing main flame front. Chemical kinetics study is also carried out to analyze chemical process during auto-ignition. Pressure wave is considered to play an important role in the initiation of direct detonation due to accumulation of intermediate radicals under higher pressure. Ignition delays under varying conditions are calculated according to the effects of pressure wave induction. As a result, gradient of ignition delays is observed, which might be a possible cause of detonation initialization.

Introduction

Increasing compression ratio as well as inlet air supercharging is a common method to increase the thermal efficiency of internal combustion Spark Ignition (SI) reciprocating engines. However, compression ratio of engine is limited by the occurrence of abnormal combustion such as knock and pre-ignition. Engine knock, characterized by pressure oscillation and "pinging" sound in cylinder, causes undesirable engine performance and even damages engine cylinder. It is commonly believed that knock is caused by end gas auto-ignition after spark plug ignition [1]. Some researchers also propose that flame propagation and acceleration in cylinder are also the reasons that lead to knock [2]. Despite these two different points of view, experiments showed that pressure profiles measured at different locations differ from each other during the same knocking cycle [3,4], which indicates the existence of propagation, interaction and reflection of pressure waves inside combustion chamber. Hydrogen, with low density, wide flammability limits and low minimum ignition

* *Corresponding author*. Tel./fax: +86 022 27402609.
E-mail address: whq@tju.edu.cn (H. Wei).
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energy, suffers knocking problem as well as gasoline when utilized in hydrogen-fueled internal combustion engine [5].

During flame propagation, heat generated from flame front will raise local temperature quickly thus driving hot gas compressing cooler surroundings. Usually, a pressure wave is formed before flame front and travels away from it at the speed of sound. However, in some extreme conditions, flame front accelerates to supersonic, thus driving pressure wave propagating at the same speed as flame front. In turn, the pressure wave heats unburned gas before flame front, which will maintain flame propagation speed. This coupling between flame front and pressure wave leads to Deflagration–Detonation Transition (DDT) phenomenon. The pressure peak of a detonation that could reach dozens of megapascal, corresponds to the magnitude of peak cylinder pressure during severe abnormal combustion.

Previous works focusing on flame propagation and interaction between pressure wave and flame can be divided into two main aspects: the initialization of reaction wave and its transition during propagation. The different regimes of flame front initialized by non-uniform initial conditions were first studied by Zeldovich using a one-step chemical model [6]. He discovered 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 which has the highest temperature $T(x)_{max}$, and the spontaneous reaction wave then propagates along the gradient with the speed u_{sp}:

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

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 values of u_{sp} indicate the initialization of different regimes of spontaneous reaction wave, such as detonation, deflagration and homogenous explosion. This theory was studied by many researchers using detailed chemistry and was extended to the research on abnormal combustion in engines [7–9]. As for transition during propagation, DDT process is mainly considered. Khokhlov et al. [10–12] numerically studied shock–flame interactions in reactive mixture. They found that flame generates and enhances shock waves, which in turn creates turbulence in flames, thus promoting the formation of hot spots, causing auto-ignition and DDT. Similar effects of pressure wave on flame were also observed by Molkov et al. [13]. They modeled hydrogen-air deflagration in a long tunnel, where initial pressure wave develops into a shock due to reflection by obstacles. There are also multi-dimension CFD simulations investigating engine knock, with different focuses and methods such as heat transfer and pressure oscillation [14,15]. Since engine cylinder is a closed narrow space, pressure wave would be reflected by cylinder walls several times during combustion. Therefore, the heating effect of pressure wave, the interactions between unburned gas and pressure wave, and the acceleration of flame influenced by pressure wave have to be considered when studying engine knock.

As is mentioned, previous works mainly focus on the initialization of different auto-ignition forms or the DDT process during flame propagation. Very few researchers establish a connection between the propagation of pressure wave and the transition of flame front under engine-relevant condition. This work aims to maintain the understanding of engine knock by considering auto-ignition and DDT process during combustion. Numerical simulation is carried out in a 75 mm one-dimensional domain, which has the similar radial length of combustion chamber. Two possible forms of combustion leading to knock are investigated: acceleration of flame and end gas auto-ignition under the effect of pressure wave. DDT process induced by pressure wave–flame interaction along with high amplitude pressure oscillation are observed and analyzed. In addition, chemical kinetics study under varying conditions due to induction of pressure wave is carried out, giving a better understanding of chemical process during auto-ignition.

Numerical details

Specifications of problem

Since the location and the moment of knock onset are mainly determined by inhomogeneity of temperature and concentration of gas mixture that result in different ignition delays, the knock is a stochastic phenomenon, which has to be studied with simplification and assumption. In this study, combustion chamber at Top Dead Center (TDC) is simplified to a 75 mm one-dimensional domain. Adiabatic boundaries are assumed to rule out heat loss to the walls. Study on mesh convergence is performed within several empirical cell sizes, at last a cell size of 0.05 mm is chosen in consideration of both the ability to capture flow discontinuity and the reduction of computational cost. Fig. 1 shows two hypotheses of flame acceleration. If the mixture is ignited at left end and propagates to the right, pressure wave that travels faster than flame front will gradually raise the temperature of whole unburned mixture during its propagation and reflection between left and right walls. As the flame speed as well as mixture reactivity increases, the propagating flame will finally transited into a detonation if some critical conditions are reached. The other hypothesis is similar to the former one but includes end gas auto-ignition. Mixture is ignited near the middle of the domain, thus forming pressure waves towards both ends that cause pressure wave-induced auto-ignition at left end. Pressure wave initialized by auto-ignited flame then propagates to the right and interacts with main flame front, leading to detonation. In fact, the occurrence of auto-ignition does not necessarily cause severe pressure oscillation, indicating that some certain critical conditions have to be reached. Since auto-ignition happens in hot spots, different temperature gradients will be formed depending on turbulence, initial thermodynamic status and heat transfer with cylinder wall and so on, thus causing different levels of knock, which is consistent with gradient theory studied by many researchers. Ignition is achieved by patching a 2 mm-thick hot zone with