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Interactions of flame propagation, auto-ignition and pressure wave during knocking combustion

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ABSTRACT

Using one-dimensional numerical simulation, the interactions of flame propagation, auto-ignition and pressure wave during various knocking combustion scenarios are systematically investigated, for stoichiometric H_2–air mixture fueled in a closed constant volume reactor. Different types of auto-ignition and pressure mutation are identified with various initial temperatures. It is found that as initial temperature increases, there is a transition for the auto-ignition (AI) position from the near-wall region to the region ahead of SI flame front, resulting in distinct pressure mutation and knocking intensity. Further analysis on sequential knocking combustion demonstrates that knocking intensity not only corresponds to the initial auto-ignition events induced by thermal inhomogeneity, but also to the subsequent interactions of flame front propagation, as well as AI spots initiation and pressure wave generation. Consequently, more intense pressure mutation could result from the developing detonations. Finally, the mechanism of AI occurrence and AI development is identified, which demonstrates the essential role of pressure wave disturbance in the formation of thermal inhomogeneity and detonations.

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1. Introduction

Recently engine downsizing with supercharging technology has become increasingly attractive in spark-ignited (SI) engines because of its higher thermal efficiency and lower emissions [1]. However, the required increments in Brake Mean Effective Pressure (BMEP) induce severe thermodynamic conditions, which promote the possibilities of abnormal combustion phenomena prior to or during engine combustion, such as knock or super-knock [2–3], both of which are supposed to be induced by auto-ignition (AI) events during premixed combustion. Auto-ignition originates from a single or multiple hot (or cold) spots by which a combustible mixture reacts in a self-accelerating manner, and eventually becomes explosive, leading to fully fledged combustion followed by intense pressure mutations [4]. Although extensive numerical and experimental work has been done, there is still lack of understanding on the generation of the strong pressure wave during knocking combustion and the process of detonation development in such limited space during engine combustion [5].

Recent study on knocking combustion can be traced to the flame propagation and end-gas auto-ignition with thermal and concentration stratifications in the charge. A pioneering work by Zel'dovich [6] pointed out that there are different combustion modes for a flame front propagating in the charge with non-uniform reactivity. Later, Bradley, Gu and Kalghatgi [7–9] developed a theoretical relation based on a group of dimensionless parameters (ξ, ε), representing the normalized temperature gradient and the ratio of acoustic time to excitation time respectively, to describe the limits of developing detonation mode based on H_2–CO–air and H_2–air mixtures. Griffiths [10] and Dai et al. [11] studied the negative temperature coefficient (NTC) behavior of end-gas auto-ignition, suggesting the essential role of AI heat release and pressure wave in subsequent evolution of combustion behaviors. However, due to the artificially introduced temperature gradients and lack of modeling SI flame propagation, the influence of flame front propagation on end-gas auto-ignition and their interactions have been neglected in most of these investigations.

To study the interactions of flame front propagation and end-gas auto-ignition, Pitz and Westbrook [12] firstly examined the transient behavior of a laminar reaction front propagating into the auto-igniting mixture near the wall region, and found that high heat release rate during end-gas auto-ignition could generate strong pressure waves. Further, Martz et al. [13–14] performed one-dimensional

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(1D) steady and unsteady numerical simulations for a laminar reaction front propagating into an auto-igniting mixture, and found that the reaction progress of end auto-igniting mixture significantly influences the combustion regime transitions of propagating flame fronts. Unfortunately, the physics related to transient pressure waves was not accounted for in their models. A numerical work by Ju et al. [15] suggested that there are at least six different combustion regimes at near NTC temperatures during the dynamic interactions between flame front propagation and end-gas auto-ignition. However, the mechanism of strong pressure wave generation and the subsequent influence on flame front dynamics was not addressed.

The interactions of flame front propagation, end-gas auto-ignition and pressure wave are very complicated but extremely crucial during knocking combustion, which affect the characteristics of local pressure mutation, combustion regime transitions and knocking intensity. Robert et al. [16] used 15 LES cycles of a high load/low speed SI engine operations to visualize the knocking and super-knocking combustion, and found that the coupling of pressure wave, AI spots and AI heat release may contribute to a deflagration to detonation transition (DDT). However, the empirical models utilized in their three dimensional (3D) simulation prevent a deeper physical understanding on the detailed processes for such interactions. A 1D direct numerical simulation was performed by Terashima et al. [17] on the pressure wave induced by the end-gas auto-ignition. However, an essential process of transient pressure mutation resulting from the flame front-wave interaction was not demonstrated. Additionally, the actual physical process for flame front propagation, end-gas auto-ignition and pressure (or shock) wave during knocking combustion spans up to 12 orders of magnitude in terms of the time scale [18], it is reasonable to utilize an advanced algorithm like adaptive mesh refinement to improve numerical fidelity and computational efficiency.

This study aims to demonstrate the underlying mechanism during the interactions of flame propagation, auto-ignition and pressure wave during knocking combustion, with special emphasis on auto-ignition occurrence and pressure mutation generation. The paper was organized as follows. Flame front initiation, propagation and AI generation in constant volume reactor filled with homogeneous stoichiometric H_2–air mixture were firstly studied under different initial temperatures to visualize various scenarios of engine knocking combustion. Then the sequential interactions of flame front propagation, auto-ignition and pressure wave were discussed, followed by analysis based on the evolution of thermodynamic conditions, different velocity scales associated with each phenomenon, and the temperature inhomogeneity. Finally, to demonstrate the essential role of pressure wave in the formation of thermal inhomogeneity and detonation wave, the effects from chamber lengths and thermodynamic states of local mixture in flame preheat zone were analyzed.

2. Methodology and models

2.1. Governing equations

In order to resolve the multi-physical problem involving flame propagation, auto-ignition and pressure wave, a time-accurate and space-adaptive numerical solver for Adaptive Simulation of Unsteady Reactive (A-SURF) is used to perform high-fidelity numerical simulations. The unsteady Navier–Stokes equations and the energy and species conservation equations for a multi-components reactive mixture in a 1D rectangular coordinate are solved in the A-SURF [19]:

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

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

$$U=\begin{pmatrix} pY_1\\ pY_2\\ \cdot\\ \cdot\\ \cdot\\ pY_N\\ pu\\ E\end{pmatrix},\ F(U)=\begin{pmatrix} puY_1\\ puY_2\\ \cdot\\ \cdot\\ \cdot\\ puY_N\\ pu^2+P\\ (E+P)u\end{pmatrix},$$

$$F_v(U)=\begin{pmatrix} -puY_1V'_1\\ -puY_2V'_2\\ \cdot\\ \cdot\\ \cdot\\ -pY_nV'_n\\ \tau\\ q\end{pmatrix},\ S=\begin{pmatrix}\omega\\ \omega\\ \cdot\\ \cdot\\ \cdot\\ \omega_n\\ 0\\ 0\end{pmatrix} \tag{2}$$

Here ρ is the density, u the flow velocity and E the total energy per unit volume, and Y_K, V'_K and ω_K are the mass fraction, diffusion velocity and production rate of specie K, respectively. The production rate of species K, ω_K, due to chemical reaction is specified via collection of elementary reactions using a CHEMKIN compatible database [20]. The mixture-averaged method is employed to calculate diffusion velocity and the Soret diffusion effect of H and H_2 is considered. In the momentum equation, P is hydrostatic pressure and τ is viscous tress tensor represented by $\tau=\mu(2S)-\frac{2}{3}\mu(\nabla\cdot u)\delta$, where μ is the viscosity of the mixture and S the symmetric strain rate tensor. In the energy conservation equation, the total energy, E, is defined through

$$E=-P+\frac{pu^2}{2}+ph,\quad h=\sum\nolimits_{K=1}^{K=n}(Y_Kh_K),$$
$$h_K=h_{(K,0)}+\int_{T_0}^{T}C_{P,K}(T)dT \tag{3}$$

where T is the temperature, h_K the enthalpy of species K, $h_{K,0}$ the species enthalpy of formation at the reference temperature T_0 and $C_{P,K}$ the specific heat of species K at constant pressure. The heat flux q is defined as

$$q=-\lambda\nabla T+\rho\sum\nolimits_{K=1}^{K=n}\left(h_kY_kV'_K\right) \tag{4}$$

where λ is thermal conductivity of mixture.

A-SURF has been successfully used in the research of auto-ignition, flame propagation, shock wave propagation and detonation combustion, and the more details on numerical schemes and code validation can be found in the paper [11,19,21–22].

2.2. Numerical methodology

During the simulations, the second-order accurate, Strang splitting fractional-step procedure is adopted in order to separate the time evolution of stiff reaction term from that of the convection and diffusion terms. In the first fractional step, the non-reactive flow is resolved and Runge–Kutta, MUSCL-Hancock and central difference schemes, all with second-order accuracy, are employed to calculate temporal integration, convective and diffusion flux, respectively. The second fractional step is to solve the chemistry term using the VODE solver. Meanwhile, a multi-level algorithm with adaptive mesh refinement has been applied based on the first-order and second-order gradient of temperature, velocity and major species distributions to guarantee adequate numerical resolutions for the propagating flame front, end-gas auto-ignition and pressure waves [23]. Moreover, a finest mesh of 1 μm and the corresponding time step is 8×10^{-11} s is utilized in the current work.

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