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LES analysis for auto-ignition induced abnormal combustion based on a downsized SI engine

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HIGHLIGHTS

- Knock and super-knock are studied using LES with detailed chemistry solver.
- Classical knocking intensity varies proportionally with spark-ignition timing.
- Low-temperature chemical reaction plays important role in super-knock formation.
- Developing detonation can be induced by multiple or single hot-spot auto-ignition.
- Developing detonation wave directly by single hot-spot produce stronger knocking.

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ABSTRACT

Engine knock and super-knock have become the main barriers to significantly improving engine thermal efficiency. To further study the nature of the abnormal combustion, this work quantitatively investigates engine knock and super-knock using a Large Eddy Simulation framework coupling detailed chemistry solver. Firstly, classical knocking cycles with different knocking intensities have been calculated through adjusting spark-ignition timing. It shows that knocking onset and intensity vary proportionally with the advance of spark-ignition timing, however, super-knock events are not observed under the operation conditions. Then for a given spark-ignition timing, the blends of Primary Reference Fuels are introduced in order to obtain different octane number of mixture, through which super-knock events with stronger knocking intensity are observed. The results show that as the decreases of octane number, knocking onset is significantly advanced due to the enhancement of low-temperature chemical reactivity. Consequently, more auto-ignition centers appear at hot exhaust valve side and even cool intake valve side at very low octane number. But for the knocking intensity, it does not always show a proportional correlation with octane number during super-knock. Further auto-ignition scenarios show that developing detonation wave can be induced by both multiple hot-spots auto-ignition and directly by single hot-spot auto-ignition, with different reaction front curvatures. However, the later seems to produce much stronger knocking intensity, especially when there are several developing detonation waves during super-knock. Therefore, how to effectively regulate local auto-ignition initiation and development seems the key to the avoidance of abnormal combustion in modern engines.

1. Introduction

Nowadays highly boosted spark-ignited (SI) engines show great advantages in the improvement of thermal efficiency. However, the risk of abnormal combustion, e.g. classical knock and super-knock, may often be encountered when the engine is operated under high-load conditions [1]. Engine knock is generally considered as a result of end-gas auto-ignition before the arrival of main flame front [2], and super-knock is attributed to a developing detonation due to the resonance between acoustic wave and reaction wave in multi-scale turbulent flows. When super-knock occurs, stochastic auto-ignition reaction fronts may consume surrounding mixture within less than a millisecond, which can cause a knocking intensity beyond 20 MPa [3]. Despite the numerous studies devoted to the abnormal combustion [4–7], there are still many ambiguities associated with the key physical–chemical mechanisms, which hinder the rapid development of modern SI engines.

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For a long time, the visualization experiment has been considered as an important access to the fundamentals of abnormal combustion thanks to its capability in capturing microcosmic mechanism of combustion processes [8]. Based on an optical hydrogen SI engine, Kawahara et al. [9] found that end-gas auto-ignition and subsequent pressure wave in knocking combustion could be visualized through a high-speed camera. Using chemiluminescence imaging technology, Vafamehr et al. [10] investigated the competing chemical and physical effects of transient fuel enrichment on heavy knock in an optical SI engine. Through high-speed direct photography, Wang et al. [11] experimentally analyzed the events of pre-ignition and super-knock in a rapid compression machine, and possible mechanism for super-knock formation was obtained. Despite the wonderful visualization work, wide applications of the visualization techniques in knocking combustion are still difficult due to the limitations in both engine systems and measuring methods.

Compared with visualization experiments, Computation Fluid Dynamics (CFD), especially Large Eddy Simulation (LES), has become attractive to the study of abnormal combustion [12]. This is because the LES allows for the stochastic behavior of individual cycles and the variations of multiple cycles [13]. Based on a new LES framework coupling flame surface density model and tabulated kinetics, Lecocq et al. [14] found that the local auto-ignition initiation and development, consistent with in-cylinder pressure history, could be accurately captured during SI engine knock. Using dual heat transfer and two-step reduced scheme, Misdariis et al. [15] carried out a LES work to explore the effect of transient temperature distributions on engine knock, and found that local auto-ignition largely depends on the temperature heterogeneity in cylinder. Several numerical studies on classical knock have been performed, however, there is few LES literature focusing on the formation of super-knock under practical engine conditions.

Theoretically both classical knock and super-knock are induced by local sporadic auto-ignition phenomena. Rudloff et al. [16] experimentally investigated the relation between pre-ignition and super-knock in terms of auto-ignition initiation and development. They found that early pre-ignition only tends to vary surrounding thermodynamic conditions, and it is the later gaseous auto-ignition at other regions contributing to the eventual super-knock. Bradley et al. [17] pointed out that the developing detonation within a multitude of hot spots would be very damaging, and as the number of hot spots increases, so do the interactions between adjacent ones. Using 15 LES cycles of a high load/low speed SI engine operating point, Robert et al. [5] analyzed deflagration to detonation mechanism, and found that one or a couple of hot spots are strong enough to induce local temperature increases, which further promotes the coupling between pressure wave and auto-ignition reaction rate and eventually the formation of super-knock. Therefore, it is necessary to further explore physical–chemical mechanism of local hot-spots auto-ignition during abnormal combustion, the results of which will provide effective approaches to the optimization of engine combustion.

The primary objectives of current numerical investigations are to further explore the role of local sporadic auto-ignition and fuel property in both classical knock and super-knock based on a highly downsized SI engine. Classical knocking cycles were obtained through the advance of spark-ignition timing, and super-knock events were achieved by decreasing octane number of Primary Reference Fuels (PRF). Current LES numerical investigations will give insights into the ways how to effectively restrain the occurrence of abnormal combustion in modern engines, such as exhaust gas recirculation and water injection technology [18,19].

2. Methodology and model descriptions

2.1. SAGE detailed chemistry solver

To accurately predict the sporadic auto-ignition controlled by chemical kinetics, a SAGE detailed chemistry solver [20] was adopted in CONVERGE CFD code [21]. The SAGE solver calculates reaction rate of each elementary reaction while CFD code solves transport equations. Combined with the algorithm of Adaptive Mesh Refinement (AMR), a detailed mechanism can be used to simulate various combustion regimes, including ignition, premixed and mixing-controlled combustion, etc. Therefore, the SAGE solver is perfect for these numerical simulations related to auto-ignition controlled combustion processes.

As described by Turns [22], a multi-step chemical reaction mechanism can be written in:

$$\sum_{i=1}^{M} \nu'_{i,r}\chi_i = \sum_{i=1}^{M} \nu''_{i,r}\chi_i \quad r = 1,2,\ldots,R \tag{1}$$

where $\nu'_{i,r}$ and $\nu''_{i,r}$ are the stoichiometric coefficients for reactants and products, respectively, for species i and reaction r, R is the total number of reactions and χ_i represents species i.

Net production rate for species i can be obtained by:

$$\dot{\omega}_i = \sum_{r=1}^{R} \nu_{i,r} q_r, \quad i = 1,2,\ldots,M \tag{2}$$

where M is the total number of species, $\nu_{i,r} = \nu''_{i,r} - \nu'_{i,r}$.

The rate-of-progress variable q_r for the rth reaction is:

$$q_r = k_{fr}\prod_{i=1}^{M}[X_i]^{\nu'_{i,r}} - k_{br}\prod_{i=1}^{M}[X_i]^{\nu''_{i,r}} \tag{3}$$

where $[X_i]$ is the molar concentration of species i, and k_{fr} and k_{br} are the forward and reverse rate coefficient for reaction r.

The governing equations of mass and energy conservation can be solved for a given computational cell:

$$\frac{d[X_i]}{dt} = \dot{\omega}_i \tag{4}$$

$$\frac{dT}{dt} = \frac{V\frac{dP}{dt} - \sum_m (h_i \dot{\omega}_i)}{\sum_m ([X_m]\bar{c}_{p,i})} \tag{5}$$

where V is volume, T temperature, P pressure and $\dot{\omega}_i$ net reaction rate of species i. The h_i and $\bar{c}_{p,i}$ are the molar specific enthalpy and molar constant-pressure specific heat, respectively.

The above equations are solved at each CONVERGE computational time-step, and cell temperature is updated after chemistry calculation is converged. To expedite the detailed chemistry, a minimum cell temperature T_{cut} and minimum hydrocarbon mole-fraction HC_{min} are specified, below which the kinetics are not solved.

2.2. One-equation Eddy viscosity model

A one-equation sub-grid scale (SGS) eddy viscosity model [23,24] has been used to solve a sub-filter-scale (SFS) kinetic energy transport equation, and turbulent viscosity is modeled by employing the SFS turbulent kinetic energy and filter size. Due to the good performance in adapting various grid levels, this model has been widely used to resolve complex flow filed.

The sub-grid kinetic energy equation is given by:

$$\frac{\partial k}{\partial t} + \bar{u}_i\frac{\partial k}{\partial x_i} = -\tau_{ij}\frac{\partial \bar{u}_i}{\partial x_n} - \varepsilon + \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial x_i}\right) \tag{6}$$

where the sub-grid kinetic energy is given by: