Effect of turbulent mixing on the end gas auto-ignition of *n*-heptane/air mixtures under IC engine-relevant conditions

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A B S T R A C T

The effect of turbulence on the end-gas auto-ignition (AI) of stoichiometric *n*-heptane/air mixtures under engine relevant conditions is numerically studied through a combined methodology of Large Eddy Simulation (LES) and one-dimensional stand-alone Linear Eddy Model (LEM). Similar end-gas auto-ignition process in super rapid compression machine experiments is first been qualitatively reproduced through LES. To further investigate the effect of small-scale turbulence-chemistry interaction on the end-gas auto-ignition in the near-wall region which consists of a core region and a boundary layer, 1-D LEM simulations are performed by extracting the thermal-chemical and turbulent parameters at top dead center from LES. The parametric study covers a range of representative fluctuation velocity values under engine-like conditions at two initial temperatures of 700 K and 900 K, which are below and within the Negative Temperature Coefficient regime respectively. It is generally found that, increased turbulence intensity delays AI formation and also reduces the kernel size at the onset of AI. At the initial temperature of 700 K, intense turbulence can change the combustion mode of the end-gas following the initial spontaneous auto-ignition in the core region. Diffusive - reactive flame structures are observed and the kernel expansion is governed by turbulent flame propagation. At a high initial temperature of 900 K, the formation of "cold" AI kernels is inhibited with increased turbulence intensity. A budget analysis reveals that the expansion processes of nascent kernels mainly are spontaneous ignitions and turbulence may enhance the local scalar mixing. However, turbulence won't change the nature of auto-ignition propagation wave driven dominantly by exothermicity during the end-gas combustion process.

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1. Introduction

End-gas auto-ignition (AI) before a deflagration flame could induce a subsequent rapid heat release which can lead to a localized destructive pressure pulse. This may occur during the combustion process of Internal Combustion (IC) engines, such as spark ignition (SI) and spark-assisted compression ignition (SACI) [1,2]. Thus, the end-gas reaction process could be a key factor influencing combustion process. However, a comprehensive understanding of the physiochemical processes in the formation and nascent expansion of the AI kernels under realistic engine conditions is challenging due to the complicated chemical kinetics of heavy hydrocarbon fuels, its sensitivity to possible thermal distribution and state of un-

burnt mixture, and the turbulence-chemistry interaction (TCI) involved [3,4].

The Negative Temperature Coefficient (NTC) phenomenon and the consequent multi-stage ignition characteristics of heavy hydrocarbon fuels significantly complicate the end-gas ignition process [5]. For conventional IC engines, the mean temperature of fresh charge inside the cylinder at Top Dead Center (TDC) is typically within the range of 600–1000 K, which overlaps with the NTC regime. Although the heat released from low-temperature reactions (LTR) at the first ignition stage can be relatively low, a non-negligible effect on the second ignition stage can also be found as reported in Ref. [6]. Furthermore, due to the non-monotonic dependence of ignition delay time with the temperature within NTC regime, AI kernels may initially form in low temperature regions, in the boundary layers. These exothermic centers are called "cold spots" which are crucial for the end-gas auto-ignition process and the potential engine knock [5–7].

Besides complex chemical kinetics, the thermal distribution and the state of fuel/air mixture will also affect the AI kernels

expansion. This process may be dominantly driven by the pre-flame spontaneous exothermic reaction of the ending gas or by the premixed front, controlled by the heat transport from products to reactants. Recent simulations of Dai et al. [8] identified various auto-ignition propagation modes of *n*-heptane/air mixtures, such as deflagration, detonation, shock-detonation, and shock-deflagration when imposing different temperature gradients in a one-dimensional planar configuration. Hajireza et al. [9] numerically investigated the expansion of AI kernels with a detailed Primary Reference Fuel (PRF) mechanism. A negative correlation between the temperature gradient and the auto-ignition flame speed was found and attributed the reduced tendency of the formation of auto-ignition flame propagation with a nearly homogeneous temperature distribution. To clarify the mechanism in the spread of auto-ignition, Martz et al. [10,11] explored the effect of unburnt mixture reaction progress on the flame propagation in *iso*-octane/air mixture, under SACI operating conditions. The result showed that the diffusive–reactive balance of a flame front gradually disappears when reaching a certain level of end-gas reaction progress. Then, the pre-flame spontaneous reaction of the ending gas dominates the propagation resulting in a rapid auto-ignition spread.

Note that most theoretical and numerical studies reported in the literature do not consider the effect of TCI on the end-gas ignition process which is in general non-negligible. DNS studies [12–14] revealed that with the increased fluctuation velocity together with a deceased turbulence time scale the overall combustion in an HCCI engine fueled with *n*-heptane is retarded and leads to a more rapid and homogeneous auto-ignition. More recently, Kim et al. [15] quantified the effect of turbulence by using the ignition Damköhler (Da) number. It is shown that under high pressure and intermediate temperature, the propagation of the auto-ignition flame, which has similar characteristics with the premixed front propagation, is controlled by the heat transfer from the products to the reactants and intense turbulence could advance the overall combustion by increasing the flame surface area. These previous studies on HCCI illustrate the importance of TCI during the combustion process and reveal that TCI effects depend on specific operation conditions. Unfortunately, relevant works are still very limited due to the high computational cost of DNS. In addition, the effect of turbulence on low-temperature combustion is worth further study.

The present work aims to provide insights into the effect of turbulence on the end-gas auto-ignition process under IC engine-relevant conditions. Particular focus is on the end-gas ignition in the near-wall region with a temperature gradient in the boundary layer. The n-heptane is chosen as the surrogate fuel considering that it is one main component of PRF for IC engines and it exhibits NTC phenomenon. In addition, the predicted combustion characteristics from large eddy simulations (LES) can be validated with the super rapid compression machine (RCM) experiments of Katsumata [16] in which n-heptane is employed. The experiment was conducted to study knock using high-speed direct and schlieren photography under engine-like thermal states. Note that, during the compression stroke, large-scale swirls and tumbles are compressed and then fragmented into small-scale (around 0.01–1 mm) turbulent eddies. The length-scale is usually below the LES grid resolution and the subgrid small-scale TCI needs modeling. In this study, an integrated approach consisting of LES and one-dimensional linear eddy model (LEM) simulations is employed to investigate the flame propagation and end-gas ignition process. A parametric study of the effects of small-scale turbulent mixing on the formation and expansion of auto-ignition kernels in the near-wall regions are performed using LEM simulations with the necessary information, such as turbulence quantities, being extracted from LES. Two typical thermal states with the initial

temperatures being below and within NTC region respectively are considered.

The rest of the paper is organized as follows. In Section 2, the LES modeling approach is first presented followed by a description of the 1-D LEM simulations. Results and key findings are reported and discussed in Section 3. Conclusions are in Section 4.

2. Methodologies

The integrated approach consisting of 3-D LES and 1-D LEM simulations is formulated for studying the ignition/flame propagation in engine as follows.

2.1. Large eddy simulations

The LES solver [17,18] in KIVA-3 V [19] is based on the arbitrary lagrangian–eulerian (ALE) method with finite volume method. Regarding the continuum phase, a third-order Monotone Upstream-centered Schemes for Conservation Laws is implemented to achieve high order accuracy for the convection term. The governing equations for the filtered quantities are

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho} \tilde{u}_i \tilde{u}_j - \bar{\tau}_{ij} + \tau_{ij}^{sgs}\right) = 0, \tag{2}$$

$$\frac{\partial \bar{\rho} \tilde{E}}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{E} \tilde{u}_j + \bar{q}_j - \tilde{u}_i \bar{\tau}_{ij} + H_j^{sgs} - \sigma_j^{sgs}) = \bar{\dot{Q}}^c, \tag{3}$$

$$\frac{\partial \bar{\rho} \tilde{Y}_s}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho} \tilde{u}_j \tilde{Y}_s - \bar{\rho} \bar{D}_s \frac{\partial \tilde{Y}_s}{\partial x_j} + \Phi_{j,s}^{sgs} + \theta_{j,s}^{sgs}\right) = \overline{\dot{\omega}_s^c}, \tag{4}$$

in which the superscripts "-" and "~" are respective the filtered and favre-filtered quantity, "*sgs*" is the abbreviation for sub-grid scale, ρ is density, u is velocity, $\overline{\dot{\omega}_s^c}$ is reaction source term for species, Y_s is the mass fraction of species s, E is the specific total energy, H is the heat flux, D_s is the diffusivity of species s, $\dot{Q}^c$ is the chemical heat release rate, Φ is the mass flux, θ is diffusive mass flux, σ_i is the viscous work and τ_{ij} is the stress tensor.

The unclosed terms in the governing equations presented in the manuscript are sub-grid stress tensor τ_{ij}^{sgs}, species mass flux $\Phi_{j,s}^{sgs}$, diffusive mass flux θ_j^{sgs}, heat flux H_j^{sgs} and unresolved viscous work σ_j^{sgs}. The sub-grid stress, τ_{ij}^{sgs} is modeled with eddy viscosity hypothesis given by

$$\tau_{ij}^{sgs} = -2\overline{\rho}\nu_t\left(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{kk}\delta_{ij}\right) + \frac{2}{3}\overline{\rho}k^{sgs}\delta_{ij}. \tag{5}$$

The turbulent kinetic energy k^{sgs} is obtained from its modeled transport equation

$$\frac{\partial \bar{\rho} k^{sgs}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j k^{sgs}}{\partial x_j} = P^{sgs} - D^{sgs} + \frac{\partial\left(\frac{\bar{\rho}\nu_t}{Pr_t} \cdot \frac{\partial k^{sgs}}{\partial x_j}\right)}{\partial x_j}, \tag{6}$$

where P^{sgs} and D^{sgs} are the sub-grid production term and energy dissipation rate term, respectively. In the RCM experiment, the fresh charge is still without turbulence. Hence, the initial value of k^{sgs} is set to 0 in LES. Pr_t is the turbulent Prandtl number. The sub-grid species mass flux $\Phi_{j,s}^{sgs}$ is obtained by the gradient diffusion closure:

$$\Phi_{j,s}^{sgs} = -\overline{\rho} \cdot \frac{\nu_t}{Sc_t} \cdot \frac{\partial \tilde{Y}_s}{\partial x_j}. \tag{7}$$

The sub-grid diffusive mass flux $\theta_{j,s}^{sgs}$ is ignored, since this term is in general small compared to $\Phi_{j,s}^{sgs}$. Note that, since specific internal energy equation is adopted here instead of total energy equation. The subgrid heat flux H_j^{sgs} and viscous work σ_j^{sgs} are not