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A DNS study of the ignition of lean PRF/air mixtures with temperature inhomogeneities under high pressure and intermediate temperature

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ABSTRACT

Two-dimensional direct numerical simulations (DNSs) of ignition of lean primary reference fuel (PRF)/air mixtures at high pressure and intermediate temperature near the negative temperature coefficient (NTC) regime were performed with a 116 species-reduced mechanism to elucidate the effects of fuel composition, thermal stratification, and turbulence on PRF homogeneous charge compression-ignition (HCCI) combustion. In the DNSs, temperature and velocity fluctuations are superimposed on the initial scalar fields with different PRF compositions. In general, it was found that the mean heat release rate increases slowly and the overall combustion occurs rapidly with increasing thermal stratification regardless of the fuel composition. In addition, the effect of the fuel composition on the ignition characteristics of PRF/air mixtures was found to be significantly reduced with increasing thermal stratification. Chemical explosive mode (CEM) and displacement speed analyses verified that nascent ignition kernels induced by hot spots due to a high degree of thermal stratification usually develop into deflagration waves rather than spontaneous auto-ignition at reaction fronts and as such, the mean heat release rate becomes more distributed over time. These analyses also revealed that the fuel composition effect vanishes as the degree of thermal stratification is increased because the deflagration mode of combustion, of which propagation characteristics are nearly identical for different PRF/air mixtures, becomes more prevailing with increasing degree of thermal stratification. Ignition Damköhler number was proposed to quantify the successful development of deflagration waves from nascent ignition kernels; for cases with large ignition Damköhler number, turbulence with high intensity and short timescale can advance the overall combustion by increasing the overall turbulent flame area instead of homogenizing initial mixture inhomogeneities.

1. Introduction

The fundamental ignition characteristics of various fuel/air mixtures under lean, dilute, elevated pressure, and relatively low temperature have been widely investigated due to their practical relevance to homogeneous charge compression-ignition (HCCI) engine combustion [1–14]. An HCCI engine and its many variants have been considered as one of the most probable alternatives to the conventional internal combustion engines due to its potential to provide high diesel-like efficiency with very low pollutant emissions [1–14]. However, the development of prototype HCCI engines remains challenging because of their significant drawbacks in preventing an excessive pressure rise rate (PRR) under high-load conditions and controlling precise ignition timing of HCCI combustion. In general, the excessive PRR occurs due to volumetric auto-ignition throughout an HCCI engine cylinder. Moreover, HCCI engines have no explicit ignition method such that ignition timing in HCCI combustion is primarily governed by the chemical kinetics of fuel/air mixture, which strongly depend on the overall mixture composition, temperature, and pressure. Therefore, there have been many attempts to control the ignition timing and to alleviate the excessive PRR in HCCI combustion by applying different fuel injection, fuel preparation, and thermal management strategies including exhaust gas recirculation (EGR) [1–14].

Several computational studies of HCCI combustion using multi-dimensional direct numerical simulations (DNSs) have been conducted to elucidate the fundamental combustion characteristics of various fuel/air mixtures under HCCI conditions including hydrogen [15–19], dimethyl ether (DME) [20,21], *n*-heptane [22], *iso*-octane [23], primary reference fuel (PRF) [24], ethanol [25], and biodiesel [26]. From these studies, the general characteristics of HCCI combustion have been elucidated; thermal stratification in an HCCI engine cylinder can spread out the PRR under high-load

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conditions by changing the combustion mode of spontaneous auto-ignition into a mixed combustion mode of spontaneous auto-ignition and deflagration [15–18,22,23]. In the presence of large temperature fluctuations, auto-ignition of hotter mixtures first occurs and evolves into deflagration waves, which spread to the unburnt mixtures sequentially until the remaining charge auto-ignites simultaneously. In general, the speed of the deflagration waves is much less than that of the spontaneous auto-ignition fronts and hence, the overall combustion is temporally spread out, resulting in a reduction of peak PRR.

In many previous DNS studies [15–19], the ignition characteristics of hydrogen/air mixtures exhibiting only one-stage ignition were investigated and as such, the effect of the negative-temperature coefficient (NTC) regime on HCCI combustion was not appreciated. The NTC regime usually appears as a result of the low-temperature oxidation of large hydrocarbon fuels exhibiting two-stage ignition. The effect of the NTC regime on HCCI combustion was first investigated by Yoo et al. [22] using 2-D DNSs of the ignition of a lean *n*-heptane/air mixture with different means and root-mean-squares (RMSs) of temperature. Recently, El-Asrag and Ju [20,21] investigated the effects of EGR and temperature/mixture stratification on the ignition of synthetic DME by adding H_2O_2 and NO to the initial mixtures. Bansal and Im [18], and Bhagatwala et al. [25] also investigated the effect of the equivalence ratio fluctuations on HCCI combustion and found that equivalence ratio fluctuations enhance HCCI combustion together with temperature fluctuations when they are uncorrelated and retard it when negatively correlated.

It is of interest to note that in a previous DNS study of the ignition of PRF/air mixtures at elevated pressure and high temperature [24], it was found that the effect of different fuel composition on the overall combustion vanishes with increasing temperature inhomogeneities. This is primarily attributed to the predominant deflagration mode of combustion at the reaction fronts and the nearly-identical propagation characteristics of different PRF/air deflagration waves. It was also found that turbulence with large intensity and short timescale can effectively homogenize the initial mixtures, rendering the overall combustion to occur by spontaneous auto-ignition.

However, the homogeneous ignition delay of different PRF/air mixtures under high pressure and intermediate temperature conditions, which are more relevant to practical HCCI combustion, shows a big disparity among the mixtures (see Fig. 1) and hence, it may be expected that the effect of fuel composition may not vanish even with large temperature fluctuations. Moreover, the early phase of ignition of a fuel/air mixture with very large temperature fluctuation may not be affected by turbulence [23]. In many previous studies [16,17,19,22–24], it was found that turbulence is likely to homogenize the initial mixtures in HCCI combustion and hence, retard its overall combustion. On the contrary, it was also found [23,25] that turbulence may enhance the overall spark-assisted compression ignition (SACI) combustion. These DNS results imply that the effect of turbulence on HCCI/SACI combustion may be inconclusive.

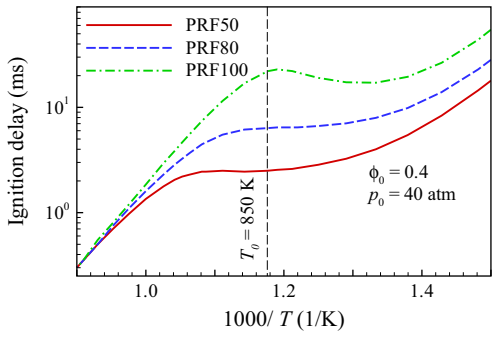

Fig. 1. 0-D ignition delay as a function of initial temperature for different PRF/air mixtures at $p_0 = 40$ atm and of $\phi_0 = 0.4$.

Therefore, the objective of the present study is to understand and compare the ignition characteristics of different PRF/air mixtures at high pressure and intermediate temperature near the NTC regime. For this purpose, we perform 2-D DNSs by varying three key parameters: (1) the fuel composition, (2) the initial temperature fluctuation, and (3) the initial turbulence intensity. Note that both the initial temperature and composition fluctuations play an important role in HCCI combustion [10,26]; in general, the equivalence ratio fluctuations enhance HCCI combustion together with temperature fluctuations when they are uncorrelated and retard it when negatively correlated. In the present study, however, we focus only on the effects of temperature fluctuations and turbulence rather than that of equivalence ratio fluctuations because large equivalence ratio fluctuations may be equivalent to large temperature fluctuations if the initial temperature of the mixture is near or above the NTC regime. Note that PRF is a fuel mixture of pure *n*-heptane and *iso*-octane; for instance, PRF80 is comprised of 80% *iso*-octane and 20% *n*-heptane by liquid volume.

2. Numerical methods and initial conditions

For the present DNSs, the Sandia DNS code, S3D [27,28], is used with a 116-species PRF/air reduced chemistry [24]. S3D solves the compressible Navier–Stokes, continuity, total energy, and species continuity equations using a fourth-order, low storage, explicit Runge–Kutta method for time integration [29] and an eighth-order central differencing scheme for spatial discretization [30] with a tenth-order filter. CHEMKIN and TRANSPORT software libraries are linked with S3D to calculate reaction rates and thermodynamic and mixture-averaged transport properties. Details of the numerical algorithm and its implementation are provided in [27]. As in previous DNS studies of HCCI combustion [22–24,26], periodic boundary conditions are applied in all directions and as such, ignition of PRF/air mixtures occurs at constant volume.

The skeletal and reduced mechanisms for PRF oxidation were developed for a previous DNS study of ignition of PRF/air mixtures under HCCI condition [24] based on the detailed LLNL mechanism [31,32], using a strategy combining directed relation graph (DRG)-based methods, isomer lumping, and timescale analysis [24,33–36]. The skeletal and reduced mechanisms were validated under various PRF composition, pressure, and temperature conditions. Readers are referred to [24] for details of the reduced mechanism.

For all DNSs, we adopted the initial uniform equivalence ratio, ϕ_0, of 0.4, pressure, p_0, of 40 atm, and mean temperature, T_0, of 850 K, respectively. p_0 of 40 atm and T_0 of 850 K represent high pressure and intermediate temperature near the NTC regime to approximate the conditions in a hydrocarbon-fueled HCCI engine at top dead center. Under the present initial conditions, the homogeneous ignition delay, τ_{ig}^0, of PRF50 and PRF80 is found to be 2.5 and 6.3 ms, respectively. Henceforth, τ_{ig} represents the time at which the maximum mean heat release rate (HRR) occurs for all simulations. The superscript 0 denotes the 0-D simulation. A total of ten different DNSs were performed in two dimensions by changing the initial physical conditions: different fuel compositions; temperature fluctuation RMS, T'; and turbulence velocity fluctuation, u'.

The initial turbulent flow field is prescribed by an isotropic kinetic energy spectrum function as in [15–17,37–39]. The most energetic length scale of turbulence, l_e, is 1.25 mm. Note that the largest velocity fluctuations in real engines are about 5 m/s such