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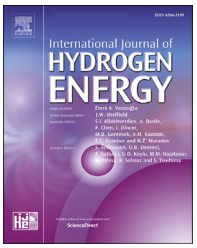

Ignition kinetics of a homogeneous hydrogen/air mixture using a transient hot jet

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ABSTRACT

The ignition characteristics of a homogenous hydrogen/air mixture using a hot transient jet generated by the combustion of syngas (H_2/CO) with varying CO concentrations from 33% to 95% in a pre-chamber is numerically investigated with particular attention to the chemical kinetics. Detailed reaction mechanism for hydrogen and syngas mixture oxidation with 15 species and 41 reactions is employed. The hot jet ignition delay time is determined by the onset of OH^* radicals and found to increase with increasing CO molar fractions in the pre-chamber fuel, and this increase is more profound for high CO content. The radicals that formed in the main chamber are examined separately from the radicals within the hot jet. Their temporal evolutions reveal that O and OH radicals in the jet play a crucial role in abstraction of H atoms form H_2/air mixture in the main chamber, which initiates ignition. Further analysis of the H_2O_2 rate of change identifies two ignition regimes. For high temperature ($T > 1000$ K) hot jets, ignition is caused by the chain branching reaction $H + O_2 \leftrightarrow O + OH$ directly, resulting in short ignition delay times (0.14, 0.19, 0.26 ms). For low temperature ($T < 1000$ K) hot jets, ignition is dominated by the accumulation and decomposition of H_2O_2, resulting in long ignition delay times (0.4, 0.67, 1.26 ms). By separating the thermal and chemical effects of the hot jet, it is found that the thermal effects are dominant but composition of the hot jet has little effect on the ignition characteristics.

Introduction

Hot turbulent jet ignition as an advanced ignition technology can potentially overcome the problems associated with lean burn combustion [1]. The problems include difficulty of ignition, slow burning speed and poor combustion stability, which may lead to partial burning, misfire and undesirable cycle-to-cycle variability [2,3]. Under the premise of successful ignition and complete combustion, lean burn combustion can reduce NOx emissions while maintaining high fuel efficiency [4,5]. In a hot turbulent jet ignition system, a small-volume pre-chamber is connected to the combustion chamber through one or several small-diameter orifice(s). The mixture in the pre-chamber is ignited by a spark plug and the burning gas is subsequently ejected into the main chamber due to the rapid increase of the pressure in the pre-chamber, resulting in a hot turbulent jet. Several studies have supported that hot jet ignition extents the lean burn limit [6–9] and increases burn rate [10–12] compared with the traditional spark ignition. However, the physics and chemistry behind the hot turbulent jet ignition are rather complicated because the jet ignition is a

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highly transient and local process which is influenced by the turbulence, hot jet temperature, radical reactions and ignition kinetics of the specific fuels.

The hot jet ignition of several kind of fuels has been studied. For the ignition of propane, Yamaguchi et al. [13] experimentally investigated the hot jet ignition mechanisms and categorized the ignition into four patterns, i.e., chemical chain ignition, composite ignition, flame kernel torch ignition and flame front torch ignition. Thelen et al. [14,15] numerically investigated the effects of pre-chamber spark location and air-fuel ratio on hot jet ignition delay time and burn rate. Gentz et al. [11,16] experimentally studied the effect of orifice diameter on the ignition by using combustion visualization in a rapid compression machine. For the ignition of natural gas using a hot turbulent jet, Gholamisheeri et al. [10,17] performed CFD modelling using both Renormalization Group (RNG) $\kappa-\varepsilon$ and Large Eddy Simulation (LES) turbulence models to investigate the jet temperature, turbulence kinetic energy and pressure traces with carefully selected chemical mechanisms. Attard et al. [7] investigated the performance, efficiency, emissions and combustion effects of turbulent jet ignition system operated in a spark ignition engine. Shah et al. [18–20] studied the effects of pre-chamber volume and nozzle diameter on the ignition characteristics in a heavy duty engine both experimentally and numerically. Reddy et al. [21] numerically investigated the effects of temperature, size and equivalence ratio of the ignition kernel on the flame development in a initially quiescent chamber under the conditions of a hot jet ignited natural gas engine. They also numerically studied the ignition kernel development in a gas with rotating vortex and examined the effects of kernel-vortex interaction on flame surface area [22]. For iso-octane, Gentz et al. [12] conducted experimental studies on the effects of auxiliary fuel injection using liquid propane and iso-octane and nozzle geometry on the ignition in an optically accessible rapid compression machine.

Because hydrogen is a promising alternative fuel and it is a simple fuel that can facilitate the fundamental investigation [23–25], several studies on ignition of hydrogen/air mixture using a hot turbulent jet have also been conducted previously. Boretti et al. [26,27] carried out a model of a direct injection jet ignition gas engine by using STAR-CCM CFD code. Based on this model, they investigated the operation of the spark-less jet ignition pre-chamber, combustion evolution in the pre-chamber and jet ignition in the main chamber. Sadanandan et al. [28] studied the ignition of near-stoichiometric hydrogen/air mixtures by hot jet using an optically accessible combustor. They focused on the ignition location and found that it occurred not at the lateral but near the tip of the jet. Biswas et al. [29] experimentally studied the effects of pressure, temperature, equivalence ratio and orifice diameter on the jet ignition process and found two different types of ignition mechanisms, i.e., jet ignition and flame ignition. Later, Biswas et al. [8,9] conducted experiments and simulations to study the effects of nozzle geometry on ignition probability. They discovered that the high-temperature zone downstream of the shocks caused an extension of the main chamber lean flammability limit. Recently, they also studied ignition of ultra-lean premixed hydrogen/air using multiple hot jets and found that the ignition probability improved near the lean flammability limit compared to the single jet [30]. Wu et al. [31] experimentally investigated the combustion characteristics of air-hydrogen mixture in an optical constant volume chamber ignited by the turbulent jets induced by pre-chamber sparkplug. They determined that compared to standard ignition the jet ignition significantly increases the combustion intensity, particularly under lean regime. Carpio et al. [32] investigated the minimum jet radius required for ignition of lean and stoichiometric hydrogen/air mixtures. They found that the minimum radius was dependent on the fuel equivalence ratio and hot jet injection velocity. These studies contributed to the understanding of ignition of hydrocarbon fuels and hydrogen using hot turbulent jets. However, the physical, chemical, and mixing and transport features of hot jet ignition still remain unclear, particularly the chemical kinetics which is essential for an ignition event and subsequent flame propagations [33,34]. Hot jet ignition is a highly local phenomenon and the radical evolutions associated with ignition chemical kinetics are not experimentally measurable. Computational fluid dynamics (CFD) coupled with detailed reaction mechanism is an effective tool to provide insight understanding of the hot jet ignition kinetics.

In the present numerical study, we focus on the chemical kinetics of homogenous premixed hydrogen/air mixture using a hot transient jet generated by the combustion of syngas (H_2/CO) in a pre-chamber. CFD simulations coupled with a detailed syngas oxidation mechanism are carried out by using our CFD code based on KIVA-3V coupled with an in-house chemical solver. The computational model is carefully validated by comparing the simulation and experimental results, which agree well. Hot jet ignition delay times are determined by evaluating the temporal evolution of OH^* radicals. Chemical insights for the observed ignition are provided via inspection of radical species evolution and critical elementary reactions. In addition, the thermal and chemical effects of the hot jet on the ignition characteristics are also investigated.

Numerical approach

In this work, ignition of homogenous hydrogen/air mixture using a transient hot jet is studied. The hot jet is generated by the combustion of syngas in a pre-chamber. To describe the turbulent flow, Reynolds-averaged Navier-Stokes equations along with the modified RNG $k-\varepsilon$ model [35,36] are employed. The details of the conservation equations for mass, momentum, energy, and species can be found in the literature [37]. The equations are solved using the code based on KIVA-3V release 2 [38]. KIVA is a fortran-based code package developed by Los Alamos National Laboratory. It numerically calculates transient, two- and three-dimensional chemically reactive fluid flows as well as combustion chemistry processes. The equations are discretized using finite-difference method both in space and time.

The simulations use a 15-species and 41-reaction syngas/air detailed chemical mechanism (Kéromnès-2013) [39]. This mechanism includes an OH^* sub-mechanism to predict an accurate OH^* emission distribution, which is important for model validation because excited OH radicals are used as an optical marker in the experiment. Moreover, the performance

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