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A numerical study on effects of pre-chamber syngas reactivity on hot jet ignition

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ABSTRACT

Ignition by a pre-chamber generated hot jet is a promising technology to reduce NO*x* emissions through extending lean burn limits. However, the role of the pre-chamber fuel reactivity in the main chamber ignition still remains unclear. In the present study, effects of the pre-chamber fuel reactivity on ignition of mixture in a main chamber by the hot jet, which is generated by the combustion of syngas in the pre-chamber, are numerically investigated. In the investigation, different ratios of CO/H_2 of syngas are considered under a thermally-equal condition. CFD simulations are performed using the code based on the KIVA-3V release 2 program coupled with an in-house developed chemical solver. A detailed chemical kinetics mechanism with 15 species and 41 reactions is adopted for the hydrogen and syngas oxidation. The hot jet ignition delay time is characterized by the maximum rate-of-change of the pressure in the main chamber. For the combustion initiation process, three stages are identified: ignition stage (stage I), flame development stage (stage II), and flame propagation stage (stage III). Significant effects of fuel reactivity are only observed on stage I that the ignition delay time considerably increases with increasing CO/H_2 ratio. Further analyses of the local temperature of the hot gas and some important elementary reactions indicate that the low reaction rate of carbon monoxide oxidation (R22: $CO + OH = H + CO_2$) causes incomplete fuel conversion in the orifice due to insufficiently available time for the reactions . The fuel conversion analysis confirms that the small-diameter orifice effect is the main reason for hot jet temperature drops under low pre-chamber syngas reactivity conditions, exhibiting as inhibiting effects on stage I.

1. Introduction

Lean burn combustion strategies have the potential to reduce NO_x emission while maintaining high efficiency in engines [1–3]. However, issues related to ignition reliability and combustion stability may arise in the lean condition, resulting in misfire, partial burning and undesirable cycle-to-cycle variability [4,5]. Ignition by a transient hot jet generated in a pre-chamber can potentially overcome these problems [6,7]. The hot jet ignition system in the current study is based on the land based large-bore spark ignition (SI) engines. In the hot jet ignition process, a near-stoichiometric mixture in a small-volume pre-chamber is ignited by sparking, which leads to a rapid increase in pressure. The high pressure ejects hot gas from the pre-chamber to the main chamber through one or more small-diameter orifices resulting in a hot transient jet which initiates the ignition of the mixture in the main chamber. The ignition is controlled by mixing time scales and chemical time scales due to the volumetric behavior of ignition onset. The mechanism of the hot jet ignition process and influencing factors, such as reactivity of the pre-chamber fuel, thermal conditions of the hot gas and turbulence generated by the high-velocity jet, are still unclear. Therefore, improved understandings of the jet ignition characteristics are valuable for the successful implementation of this advanced technology.

Many studies have been conducted to investigate the mechanism of turbulent hot jet ignition process to understand the physics behind it. Yamaguchi et al. [8] experimentally investigated the mechanisms and categorized the hot jet into several patterns. Sadanandan et al. [9] investigated the ignition of hydrogen and air mixtures by a hot jet. They found that ignition in the main chamber occurs near the jet tip rather than at the lateral sides of the jet. Biswas et al. [10,11] investigated the effects of pressure, temperature, equivalence ratio, as well as orifice diameter and geometry on the jet ignition process. They observed two types of ignition mechanisms, i.e. jet ignition and flame ignition. Ghorbani et al. [12] investigated the mechanism of hot jet ignition by using a PDF/REDIM method. They determined that macro- and micro-mixing, and chemical kinetics have a profound effect on the ignition delay time and the ignition location. Validi et al. [13] fundamentally

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studied the physical processes involved in the turbulent jet ignition by using three-dimensional direct numerical simulations (DNS). They determined that the turbulent flame and flow structures are in three main zones, i.e. hot product jet, burned-mixed and flame. Qin et al. [14] numerically investigated the transient mixing and ignition mechanisms of hot jet ignition and subsequent flame propagation for natural gas in a constant volume pre-chambre ignition system by using two-dimensional DNS. They studied the chemical effect, thermal effect and enrichment effect of the hot jet on the ignition in the main chamber in detail and found that the intermediate species, OH, CH_2O and HO_2 in the jet are important due to the chemical effect, whereas major species, CH_4, CO and H_2 are important due to the enrichment effect.

In addition to the mechanism studies, many investigations with regard to the influencing factors on the hot jet ignition process have also been done. Gholamisheeri et al. [15] experimentally studied the influence of orifice diameter and mixture equivalence ratio on the jet inlet and tip speed in a rapid compression machine. Toulson et al. [16] experimentally studied the lean limit of gasoline in a hydrogen assistant jet ignition (HAJI) system when syngas is employed as the pre-chamber fuel. They determined that the level of ignition enhancement is dependent on flame speed and the generation of chemically active radicals and not solely on the energy contained in the pre-chamber fuel. Feyz et al. [17] carried out a set of simulations for jet ignition in a confined constant volume chamber (CVC) with various pre-chamber injection pressure and fuel reactivity in the CVC. They determined an ignition probability criterion which could be used to predict the possibility of ignition development. Gentz et al. [18,19] experimentally studied the effects of nozzle diameter and number on the combustion performance by visualizing combustion and pressure traces. They determined that the orifice diameter has little impact on the 10–90% burn duration. They also performed experimental studies on the effects of auxiliary fuel injection using iso-octane [20]. In their study, the air/fuel equivalence ratio of the pre-chamber was varied from 0.93 to 3.0 by varying the injector pulse width. They found that a richer mixture in the pre-chamber lead to a shorter autoignition by the hot jet in the main chamber. However, the effect of fuel reactivity by varying the fuel composition in the pre-chamber on the hot jet ignition in the main chamber has not been investigated. In the engine practice, the fuel reactivity in the pre-chamber can be controlled through an auxiliary pre-chamber fueling system. For example, similar to the work of Gentz et al. [20–22], the auxiliary fuel can be injected into the pre-chamber by the use of an injector which is installed in the pre-chamber. Various pre-chamber fuel compositions may change the active radicals and chemical kinetics which are expected to play important roles in the hot jet ignition precess.

In the present study, syngas is chosen to be the pre-chamber fuel due to its scientifically fundamental chemistry and potential as an alternative fuel. The effects of pre-chamber syngas reactivity on the ignition process is numerically investigated by fueling pre-chamber with $CO/H_2/O_2/N_2$ mixtures with different CO/H_2 ratios (33/67, 50/50, 67/33, 80/20, 90/10 and 95/5) by mole under a thermally-equal condition. CFD simulations are performed by the use of the code based on KIVA-3V release 2 program [23] coupled with an in-house developed chemical solver. A detailed chemical mechanism, Kéromnès-2013 mechanism [24], for hydrogen and syngas oxidation with 15 species is employed. The computational model is first validated. Next, the ignition delay time is defined. The influence of the CO/H_2 ratio on the main chamber combustion initiation is investigated. To further understand the effects of fuel reactivity on hot jet ignition, the local temperature of the hot gas, important chemical reactions and pre-chamber fuel conversion in the orifice volume are studied.

2. Numerical method and simulation setup

The simulation code is based on KIVA-3V release 2 [23], which can be used to calculate transient, chemically reactive fluid flows.

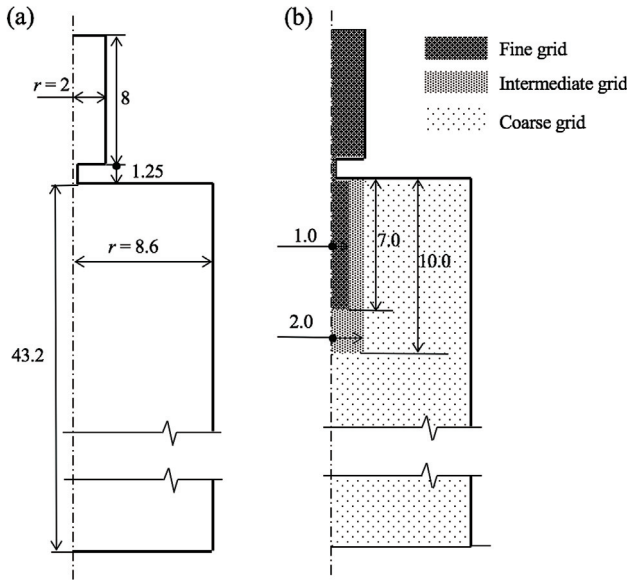

Fig. 1. Schematic sketch of the computational setup: (a) the dimensions of the computational domain, and (b) the description of fine-grid, intermediate-grid and coarse-grid regions. The dot-dosh lines refer to the axis of the geometry. The units are cm.

Reynolds-averaged Navier–Stokes (RANS) equations are solved using the KIVA code. The details of the conservation equations for mass, momentum, energy, and species can be found in literature [25]. The RANS two-equation turbulence models account for the effect of turbulence on the transportation of species, momentum and energy. Among different RANS sub-models, the $k-\omega$ models (e.g. shear stress transport $k-\omega$ model) are good for external flow predictions and boundary layer simulations [26–29]. On the other hand, the $k-\varepsilon$models, especially the Renormalization Group (RNG) $k-\varepsilon$ model, were suggested to provide appropriate results for the pre-chamber jet ignition systems [30–33]. Han et al. [34,35] have modified the RNG $k-\varepsilon$ model to account for flow compressibility to make it appreciable for internal combustion engine's simulations. In our study, the Han's RNG $k-\varepsilon$model is employed to account for the effects of turbulence in the RANS simulations.

As shown in Fig. 1(a), 2D-axisymmetric computational domain is set for a constant volume combustor by taking advantage of the symmetry. The small volume pre-chamber of 2-cm radius and 8-cm height is connected to the main chamber of 8.6-cm radius and 43.2-cm height through an orifice whose radius is 0.125 cm and a length-to-diameter ratio of 5. The computational domain is divided into three regions with different grid resolutions, shown in Fig. 1(b). Fine grids are generated in the pre-chamber, orifice and hot jet penetration region in the main chamber, since the emphasis is put on the hot jet ignition process and combustion initiation rather than on flame propagation in the main chamber.

The fine grid sizes are carefully chosen to resolve the flow field, ignition kenel and flame propagation. The smallest length scales in a turbulent flow field are the Kolmogorov scales and estimated to be of order 10^{-6} to 10^{-5} m according to the engine simulations [36]. And the laminar flame thickness is estimated to be the same as the Kolmogorov scales. The controlling processes (molecular mixing, chemical reaction) for turbulent combustion occur at these smallest scales. Hence, without a turbulence model, to resolve the turbulent combustion the grid size should be of order 10^{-6} to 10^{-5} m. In the current study, however, in the RANS turbulent field the introduced turbulent viscosity enhances mixing and eliminates the smallest scales. Thus, the length scales are significantly larger than the smallest scales. The integral length scale is estimated to be the radius of the orifice, i.e. 1.25 mm. Therefore, the cell size is chosen at the order of 0.1 to 1 mm.