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Combustion characteristics of primary reference fuels with hydrogen addition

Minye Luo, Dong Liu *

School of Energy and Power Engineering, Nanjing University of Science and Technology, Nanjing 210094, People's Republic of China

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ABSTRACT

The influences of hydrogen addition on laminar premixed fuel-rich primary reference fuels flames at atmospheric pressure are studied by the detailed kinetic analysis. The chemical effects of hydrogen addition on important intermediate species including radicals are distinguished clearly from the dilution and thermal effects. The results show that the increase of the percent of iso-octane in primary reference fuels makes the mole fractions of CH_2O and C_2H_2 reduce but facilitates the production of C_3H_3. The dilution and thermal effects of hydrogen can suppress the formation of H, O, and OH radicals and CH_2O, C_2H_2 and C_3H_3 species, and make the profiles shift to the downstream side. The hydrogen chemical effects can promote the formations of these radicals and intermediate species. The H_2 chemical effects on H radical are larger than those on O and OH radicals. The dilution and thermal effects are dominant and the overall mole fractions of H, O, and OH radicals, and CH_2O, C_2H_2 and C_3H_3 species decrease with the hydrogen addition. Finally, the detailed consumption pathways of primary reference fuels combustion with various levels of hydrogen additions are analyzed.

Introduction

The widespread use of fossil fuels has caused critical issues to societies, namely climate change and energy security. Moreover, the pollutant emissions associated with fossil fuel combustion are harmful to human health as well as the environment. In the development of the internal engine, new combustion technologies are motivated by these issues to improve combustion efficiency and reduce pollution. An accurate kinetic modeling of practical fuels is contributed to acquire a comprehensive knowledge of the physical and chemical processes occurring in combustion systems. The complexity of gasoline which contains many hundreds of different hydrocarbon species makes it impossible to obtain a detailed chemical model. It is urgent to find surrogate fuel mixtures which perform better in formulating chemical models and reproducing experiments [1]. In the present work, the primary reference fuels (PRF), n-heptane and iso-octane, are used in lieu of gasoline [2].

A large number of studies of oxidation and pyrolysis of iso-octane, n-heptane, and primary reference fuels mixtures, both experimental and numerical, have been conducted, including shock tube ignition delays [3–7], laminar burning velocity [8–10], and product species in jet-stirred reactors [11,12]. Gauthier et al. [5] measured auto-ignition times of gasoline and surrogate blends of n-heptane/toluene/iso-octane in shock tube for a variety of conditions. Huang et al. [9] experimentally analyzed the laminar flame speeds of various mixtures of primary reference fuels at atmospheric pressure via counterflow configuration and digital particle image velocimetry. Dagaut

* *Corresponding author.*
E-mail address: dongliu@njust.edu.cn (D. Liu).
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et al. [11] studied the oxidation of the primary reference fuels in the jet-stirred reactor and measured the mole fractions of reactants and main products. In numerical study, Luong et al. [13] numerically investigated the influences of thermal stratification, fuel composition, and turbulence on the ignition of primary reference fuel mixtures with a new reduced kinetic mechanism. Ra et al. [14] developed a reduced chemical kinetic mechanism of primary reference fuels which could be used to model internal combustion engines.

Hydrogen is extensively studied as a clean fuel or fuel additive since it has a high diffusion coefficient, high laminar burning velocity, wide flammability limits, low ignition energy and low emissions etc [15]. Many studies have proposed that hydrogen can be used as a fuel additive to other fuels to decrease the ignition delay [16–18], increase the laminar burning velocities [19–24], and improve the combustion efficiency and emission performances [25–31]. Hu et al. [20] experimentally and numerically studied the laminar burning velocity of premixed methane-hydrogen-air flames. The results showed that the addition of hydrogen increased the unstretched laminar burning velocity and shifted the peak value of burning velocity to the richer mixture side. Chen et al. [25] investigated the laminar premixed fuel-rich dimethyl ether flames with hydrogen addition via tunable synchrotron vacuum-ultraviolet photoionization and molecular-beam mass spectrometry. The mole fractions of major and intermediate species such as CH_2O, C_2H_2 and C_2H_4 in the flames decreased with the addition of hydrogen. Park et al. [30] elucidated the effects of H_2 addition on soot formation and oxidation in laminar premixed acetylene flames. The presence of H_2 slowed the rate of C_2H_2 oxidation and diminished the formation of benzene. Wang et al. [31] numerically studied the influences of hydrogen addition on ethylene jet flames. The mole fractions of C_2H_2 reduced greatly with the H_2 addition. The reduction of C_2H_2 which was an important precursor of soot in these researches showed that H_2 had the potential to mitigate the soot emission.

Several researches have also been conducted to study the combustion of hydrogen and hydrocarbon blends in internal combustion engines [32–38]. Akansu et al. [34] carried out a research on the performances of natural gas-hydrogen mixtures in internal combustion engines, and found that HC, CO and CO_2 emissions reduced with increasing hydrogen. Ma et al. [36] experimentally analyzed the effects of hydrogen addition on emission characteristics of a natural gas engine. The increase of hydrogen addition leaded to a reduction of unburned hydrocarbons. In 2015, An et al. [37] experimentally investigated the influence of various concentrations of hydrogen addition on the ignition delay of PRF fueled HCCI combustion, and found that the ignition delay increasing during the first-stage reaction when hydrogen was added to n-heptane. Ji et al. [38] experimentally measured the emissions of a spark-ignited gasoline engine with hydrogen addition under various loads and lean conditions. They pointed out that the hydrogen addition performed better on improving the engine efficiency and emissions performance at low load conditions. These studies showed that H_2 addition could essentially improve the performance of engine and reduce CO and HC emissions.

When gasoline or its surrogate fuel is replaced by hydrogen, the fuel mole fraction and component vary, meanwhile, the features of combustion could be subsequently changed including mole fractions of major and specific intermediate species etc. However, we don't know what really leads to these changes, either because of the reduction of fuel concentrations, or due to the addition of hydrogen. Until now, there is little work on analyzing the effects of the reactive additive H_2 in the gasoline and its surrogate fuel mixtures flames.

It is of great interest to study and understand the detailed influences of hydrogen addition on the combustion characteristics of primary reference fuels. The objective of this work is to study the detailed chemical effects of various levels of hydrogen addition on premixed laminar fuel-rich PRF (primary reference fuels) flames at atmospheric pressure under different mixture ratios of iso-octane and n-heptane. The chemical effects of hydrogen addition on the PRF combustion are distinguished and separated from its dilution and thermal effects.

Kinetic modeling and analysis method

The detailed chemical reaction mechanism we adopted for the PRF oxidation and combustion was developed by Chaos et al. [39]. It is developed to describe the high temperature pyrolysis and oxidation of iso-octane, n-heptane and their mixtures. It contains the newly updated H_2 combustion mechanism [40] and the detailed C1–C4 kinetic models [41] which present the oxidation processes of small branched species. The complete mechanism which consists of 116 species and 754 reactions has been validated against a large array of experimental data for shock tube ignition delay times, laminar burning velocities, jet-stirred and plug-flow reactors.

The modified ChemkinII/Premix code [42] is used to obtain the predictions for the freely propagated premixed laminar fuel-rich iso-octane/n-heptane/H_2/N_2 flames. The computing domain ranges from −2.0 cm at the upstream to 10.0 cm at the downstream, which is sufficiently long to achieve the adiabatic equilibrium. At the upstream, the initial temperature and pressure are set to 300 K and 1.0 atm. The equivalence ratio for all the flames keeps the same. The other detailed flame conditions are displayed in Table 1. The added hydrogen fraction (R_{H2}) is defined as the mole fraction of H_2 in the iso-octane/n-heptane/H_2 fuel blends. PRF 20 is a kind of binary fuel blends which consists of 20% iso-octane and 80% n-heptane. Similarly, PRF 50 consists of 50% iso-octane and 50% n-heptane. PRF 80 consists of 80% iso-octane and 20% n-heptane.

In order to distinguish the chemical, dilution and thermal effects [43] of hydrogen addition on iso-octane/n-heptane/H_2 flames, the following method developed by Liu et al. [28,29] is adopted here. The added H_2 is assumed as normal H_2 and fictitious H_2 (written as F−H_2). Normal H_2 can participate in all the relevant chemical reactions in flames. The fictitious H_2 owns the same thermochemical, transport data and the third-body collision efficiency with the normal H_2, but F−H_2 cannot participate in any related chemical reactions. Additionally, to keep the same equivalence ratio, part of O_2 is defined as the fictitious O_2 (written as F−O_2). Similarly with F−H_2, the F−O_2 has exactly the identical thermochemical, transport data and the third-body collision efficiency as the normal O_2, and is inert in all related chemical reactions.