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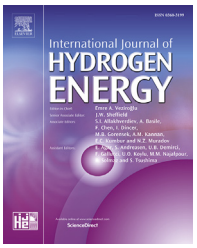

Effect of hydrogen addition on equimolar dimethyl ether/iso-octane/oxygen/argon premixed flames

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ABSTRACT

A modified one-dimensional model (Premix) in conjunction with Chemkin II and a detailed kinetic scheme combining the chemistries of hydrogen, dimethyl ether and iso-octane combustion were used to investigate the effect of hydrogen addition on the chemical composition of laminar premixed dimethyl ether/iso-octane/oxygen/argon flames. In the current modeling study, the key reaction mechanisms responsible for the observed variation in mole fractions of some major species, including radicals H, O and OH, species CO, CO_2 and CH_4 as well as oxygenated products CH_2O and CH_3CHO, were defined. The numerical modeling was focused on both chemical and dilution and thermal effects of hydrogen addition. It was found that chemical effect of hydrogen addition induced a boosting in the oxidation process whereas dilution effect led to its inhibition. The higher the hydrogen level the higher was the magnitude of the phenomenon. Besides, the chemical effect of hydrogen addition induced an enhancement in the OH, O, CO, CO_2 and CH_4 mole fractions, whereas the dilution and thermal effect led to a lowering in the amount of these species. This latter phenomenon was more important than the first effect yielding a net decrease in the concentrations of the four species. In addition, it was found that CH_2O and CH3CHO levels showed a dramatic decrease in peak height with hydrogen doping and that the contribution of the thermal effect of hydrogen addition to this lowering was more important than that of its chemical effect. Thus it can be concluded that the synergism between chemical and dilution effects played a paramount role in the dimethyl ether/iso-octane/oxygen/argon premixed flames oxidation process as well as in the rise or the decrease in the pool radicals and the major species concentrations.

Introduction

With increasing concern about depletion of crude oil resources and environmental problems, the search of using alternative fuels and developing high-efficiency combustion technology become the important issues for engine and combustion researchers [1,2]. In the first context, it was found that renewable biofuels which can be derived through biochemical processes from biomass have the potential to provide a path towards carbon-neutral fuels that are renewable and clean burning [3–5], whereas in the second context, it was reported that homogeneous charge compression ignition (HCCI) would be a potential solution technology. Dimethyl

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ether (DME), considered as a second generation biofuel [6] which can be produced from biomass as well as from natural gas and coal [7], is widely discussed as alternative fuel or additive in diesel and homogeneous charge compression ignition (HCCI) engines [8,9], gas turbines [8,10], or fuel cells [8,11]. The key properties that make the simplest aliphatic ether, DME, so attractive for compression ignition engines are its physical and combustion properties including no carbon-carbon bonds, high oxygen fraction, low carbon to hydrogen ratio, high cetane number, low boiling point, good cold-start characteristics and no air or ground-water pollution effects [1,12–14]. All these properties make dimethyl ether an excellent alternative fuel or fuel additive candidate for reducing polycyclic aromatic hydrocarbons (PAHs), NO_x, CO_2, combustion noise and emissions of particles [7,15]. Due to these promising features, extensive studies of DME pyrolysis, oxidation and combustion have been carried out in a variety of laboratory facilities including static and flow reactors [16–18], jet-stirred reactors [19–22], flow reactors [8,23–32], shock tubes [2,6,20,33–39], rapid compression machines [6,40,41] and low- and high-pressure flames [7,14,42–47].

Homogeneous charge compression ignition is a dual fuel combustion strategy leading to a potential major advance in high efficiency and low-emission engines [48]. This new strategy relies on the use of combinations of fuels with high octane and high cetane numbers [41,49,50]. In this context *iso*-octane, which is a gasoline primary reference fuel (PRF) that is highly knock resistant, with an assigned octane number of 100 [51], can be an attractive fuel candidate for use in HCCI engines. On the other hand, due to the availability of various hydrogen production systems, good combustion and favorable physicochemical properties of H_2 [52–55], the use of hydrogen as a second fuel is a widely accepted option of reducing emissions. In this context, co-combustion of hydrogen with hydrocarbons such as methane [56–60], ethylene [61,62], propane [63,64], *n*-heptane [65,66], *iso*-octane [55,67–69], and with oxygenated products such as methanol [70–73], ethanol [74–77], dimethylether [77–81], as well as with classical fuels, gasoline [82–84] and diesel [85–87], was investigated by several research groups. In all these studies, it was reported that the combustion of hydrogen/hydrocarbons mixtures exhibited several benefits as compared to that of the neat hydrocarbons.

In view of these discussions, the main purpose of this work is to numerically investigate the effect of hydrogen enrichment on the combustion of an equimolar dimethyl ether/*iso*-octane premixed flame. Chemical and dilution effects of hydrogen addition on the studied mixture behavior are highlighted.

Modeling approach

Kinetic model

The detailed chemical mechanism for DME/*iso*-octane oxidation and combustion developed by Zeng et al. [50] was used here. The mechanism containing 379 species evolved in 1931 reactions, was a combination of an *iso*-octane mechanism with diethyl ether and dimethyl ether submechanisms. The core of the reaction mechanism, used to describe oxidation and combustion of *iso*-octane, was taken from the work of Pitsch and coworkers dealing with gasoline surrogate and including submechanisms of *iso*-octane, *n*-heptane, toluene and polycyclic aromatic hydrocarbons [88]. This kinetic model has been validated against a large array of experimental data including shock tube ignition delays [89], laminar flames speeds [90] and premixed *iso*-octane flames [91]. The sub-mechanism for diethyl ether was gathered from the kinetic scheme of Tran and collaborators [92] which had been validated by using several datasets, including shock tube ignition delay times [93,94], flame speeds [95], pyrolysis experiments [94] and non-premixed flames [96]. Finally, AramcoMech2.0 sub-mechanism [97] was used for describing the dimethyl ether oxidation and combustion. It is noteworthy that the combined *iso*-octane/diethyl ether/dimethyl ether has been examined against different experiments including laminar premixed flames of *iso*-octane [91], diethyl ether [92] and dimethyl ether [98]; *iso*-octane species shock tube [99,100], ignition delay times for *iso*-octane [101,102], diethyl ether [93] and dimethyl ether [39]; laminar flame speed for *iso*-octane [103–110], diethyl ether [95] and dimethyl ether [111,112]. In addition to the examination against pure hydrocarbons, the combined mechanism was validated against premixed low-pressure flames of *iso*-octane with different amounts of dimethyl ether and diethyl ether [50].

Computational method

Calculations were performed with a modified Chemkin II/Premix code [113] with implementation of high pressure PLOG function for one-dimensional flames. Adiabatic equilibrium was kept by broadening the calculation domain from −2.0 cm at the upstream to 8.0 cm at the downstream. Averaged transport and withdraw differencing method were used for computing the *iso*-octane-DME-hydrogen-argon-O_2 freely propagated laminar premixed flames and solving the steady-state species and energy conservation equations. Computations were performed for the conditions of Zeng et al. [50]: cold gas temperature of 298 K, a pressure of 40 mbar, a mass flux of 0.003463 g/cm^2 s, an equivalence ratio of 1.53 and an equimolar composition of *iso*-octane and dimethyl ether (50%, 50%). The percentage of the relative hydrogen fraction in the fuel mixture, defined as $R_H(\%) = \frac{X_H}{X_H+X_M} x100$ where X_M is the sum of dimethyl ether and *iso*-octane mole fraction in dual fuel, and X_H the mole fraction of hydrogen, has been varied from 0 to 60 (0, 30 and 60) under fuel rich conditions.

To numerically isolate the chemical effect of hydrogen addition on the investigated flames from its dilution and thermal effects, the strategy mentioned in Refs. [77,79,114–117] was employed. The added H_2 is assumed as normal reactive H_2 and fictitious inert H_2 (referred as FH_2). Normal H_2 is allowed to participate in chemical reactions in flames, whereas the fictitious H_2 has identical thermal and transport properties as well as third-body collision efficiencies as reactive H_2 but cannot be involved in chemical reactions in flames. Thus, the observed differences between the results from the reactive and inert hydrogen additions are ascribed to the H_2 chemical effects. In order to keep the same equivalence ratio for all flames, total oxygen is divided in reactive (O_2) and

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