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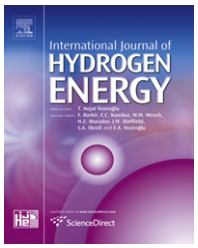

Kinetic modeling study of hydrogen addition to premixed dimethyl ether-oxygen-argon flames

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ABSTRACT

The chemical composition of flames was examined systematically for a series of laminar, premixed low-pressure Dimethyl ether (DME)-oxygen-argon flames blended with hydrogen. The effects of hydrogen addition to the DME base flame were seen to result in interesting differences. The flame is analyzed with a comprehensive kinetic model that combines the chemistries of hydrogen and DME combustion. The results indicated that the reduction of CH_3OCH_3 mole fraction in the blend is the dominant factor for the reduction of CH_3OCH_3 and CO mole fractions in the flame. The rate of the primary reactions related to CH_3OCH_3 and CO increases obviously with the addition of hydrogen. When the volume fractions of H_2 to the total of DME and H_2 exceeds 40%, H_2 will change from an intermediate species to a reactant, which means the effect of H_2 on the premixed combustion will be more significant. The free radicals in the radical pool, such as H, O and OH radicals, increase as hydrogen is added, which promote the combustion process. The mole fraction of CH_2O is decreased as hydrogen is added. Less soot precursors (acetylene (C_2H_2)) were produced with the addition of H_2.

1. Introduction

With increasing concern about fossil fuel shortage and stringent emission regulations, researches on alternative fuels gain more and more attention in the field of internal combustion engines [1,2]. As renewable energy sources with excellent characteristics, dimethyl ether and hydrogen have received considerable attention and are regarded as the most promising alternative fuels. DME is one of the most promising alternative automotive fuel solutions among the various ultra clean, renewable, and low-carbon fuels under consideration worldwide. DME can be derived from many sources, including renewable materials (biomass, agricultural products and waste) and fossil fuels (coal and natural gas). Only modest modifications are required to convert a diesel engine to run on DME [3,4]. H_2 is also being extensively studied as an excellent alternative fuel and fuel additive to spark ignition engines for its low required ignition energy, wide flammability range, high flame speed, high thermal efficiency, and low emissions [5–9].

H_2 has been used in DME homogeneous charge compress ignition (HCCI) engine to control the ignition timing and expand the load range [10]. Experimental and numerical studies of DME/air [11–13] or H_2/air premixed flames have been extensively carried out [14,15]. In the previous research, Chen et al. measured the species mole fraction profiles of DME-hydrogen-oxygen-argon laminar premixed flames by using the tunable synchrotron vacuum ultraviolet (VUV) photoionization combined with molecular-beam sampling mass spectrometry techniques [16]. Mole fraction profiles of four intermediate species including methyl radical (CH_3),

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acetylene (C_2H_2), formaldehyde (CH_2O), ethylene (C_2H_4) were measured and the effect of hydrogen addition on the combustion reaction of DME flames was analyzed.

However, constrained by the measuring technologies, only limited intermediate radicals were reported in few studies. Moreover, the combined chemical kinetics of DME and H_2 was not well understood. Since the oxidation mechanism of both DME and hydrogen are reasonably well understood, the combustion process can be simulated using chemical kinetics calculation to get comprehensive information. The objective of this study is to simulate the DME-H_2-O_2 premixed flame with detailed chemical reaction mechanism and analyze the chemical kinetics effect of hydrogen addition on the blended fuel combustion. The potential of emission reduction of DME combustion with hydrogen addition will be discussed.

2. Mechanism validation and computational methods

The detailed reaction mechanism of DME was well developed by Curran et al. [17,18]. It consists of 351 elementary chemical reactions with associated rate coefficient expressions and thermo chemical parameters for the 79 species. The detailed combustion reaction mechanism for hydrogen was included in DME oxidation mechanism.

In this study, the PREMIX code of CHEMKIN II program with detailed DME oxidation mechanism was used to calculate the DME-hydrogen-O_2 freely propagated laminar premixed flames. The PREMIX code adopts finite difference approximations and Newton algorithm technique with adaptive meshes and mixture averaged transport parameters to solve the steady-state mass, species and energy conservation equations of the calculated flames. The withdraw differencing on both convective and diffusion terms was used in the calculation. The gradient and curvature was set to be both 0.9 to control the adaptive grid. The calculation domain was from 0.0 cm at the upstream to 10.0 cm at the downstream, and this is sufficiently long to achieve the adiabatic equilibrium in the downstream. In order to compare with Chen's experiment, the initial conditions are as follows: the initial temperature is 298 K and the pressure is 4 kPa, the reactants mole fractions of the calculated flames are given in Table 1 and the mass flow rate for the solution of the freely propagated flame is to be 0.04 g/(cm^2 s). The fixed temperature to constrain the flame position is set to be 400 K. Initial guessing values of the temperature and species profiles are also assigned to start the calculation.

In order to simulate and interpret the effect of hydrogen addition on DME-O_2 premixed flame by using chemical reactions, the chemical kinetics used in the calculation must be capable of simulating pure DME and DME-hydrogen fuel blends. The comparison of the measured flame temperature of the DME-hydrogen-O_2 mixtures with the calculated results of DME oxidation mechanism is presented in Fig. 1. As the PREMIX code did not consider the heat losses (by definition) and the temperature was computed from the energy equations, the computed flame temperature is higher than that of the experiment results. As shown in Fig. 1, the flame temperature was decreased with the addition of H_2. The same effect of hydrogen addition in methane flame temperature was proven by Sepman et al. [19]. Due to the volume calorific value of H_2 was much lower than that of DME, the unit volume heat release of the mixture will decrease with the increase of hydrogen fraction. The calculation results successfully capture this behavior. This shows that the DME oxidation mechanism can well reproduce the flame temperature of DME-hydrogen-O_2 mixtures over a wide range of equivalence ratios and hydrogen fractions.

Table 1 – The reactants mole fractions of the calculated flames.

Flame no.	R(H_2)(%)	DME	H_2	O_2	Ar
1	0	0.2	0	0.4	0.4
2	40	0.1637	0.109	0.36365	0.36365
3	80	0.0857	0.343	0.28565	0.28565

3. Results and discussions

By using detailed chemical reaction mechanism, the mole fraction profiles and rate of production of all the flame species can be derived from the calculation results. Fuel-rich ($\varphi = 1.5$) DME-oxygen (O_2)-argon (Ar) premixed flames with different hydrogen fractions (volume fractions of H_2 to the total of DME and H_2 were 0%, 40% and 80%) were investigated in this study. Some representative species including the major species CH_3OCH_3, H_2, CO, the free radicals H, O, OH and C1, C2 intermediate species CH_2O and C_2H_2 are selected to analyze the effect of hydrogen addition on the DME chemical reaction.

As the mole fraction of DME is decreased with the addition of hydrogen. The calculated mole fraction of carbon-related species in the flames will be affected by this. In this study, the normalized mole fraction of the carbon-related species is used through the following formula:

$$Y_{i,n}^{N} = Y_{i,n}\frac{Y_{DME1}}{Y_{DMEn}}$$

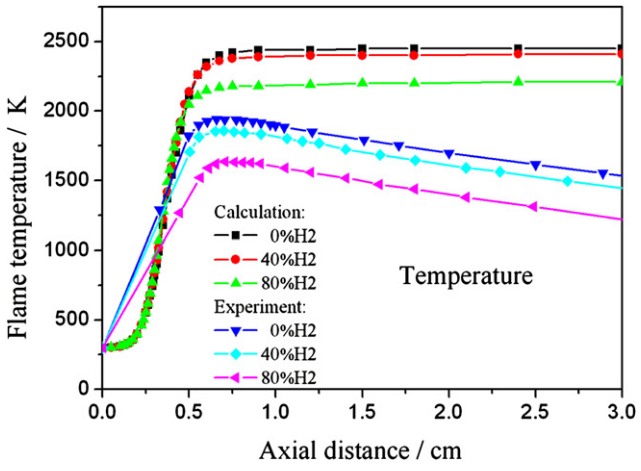

Fig. 1 – Comparison of the calculated premixed flame temperature with that of Chen's experiment [11].