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Kinetic analysis of the chemical effects of hydrogen addition on dimethyl ether flames



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ABSTRACT

The chemical effects of hydrogen addition on premixed laminar low-pressure dimethyl ether flames were studied by kinetic analysis. The chemical effects of hydrogen addition on flame structures and mole fractions of major species, intermediate species and free radicals have been distinguished clearly from the dilution and thermal effects. The results show that the chemical effects of hydrogen addition cause the DME profile to move toward the upstream side and can suppress the production of acetylene and ethylene. The production of formaldehyde is promoted by the chemical effects of hydrogen addition but the dilution and thermal effects are more dominant which decrease the mole fraction of formaldehyde so that the overall effects make formaldehyde mole fraction decrease. The dominant effects of hydrogen addition on H, OH and O radicals are the chemical effects that make mole fractions of these radicals increase.

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Introduction

As a promising alternative fuel or fuel additive, dimethyl ether (DME) has received lots of attention and research interest, since DME which can be produced from natural gas, biomass or coal, has no carbon–carbon bond, a high oxygen content, high cetane number, and low boiling point [1,2]. Several fundamental combustion chemistry studies of low-pressure DME flames have been performed using molecular-beam mass spectrometry (MBMS) in recent years [3–6]. Cool et al. [3] used a molecular-beam flame-sampling photoionization mass spectrometer with VUV synchrotron radiation (PI-MBMS) to measure the mole fractions for flame species in low-pressure premixed fuel-rich DME/oxygen/argon flat flames and compared the measured results with modeling. Wang

et al. [4] performed the comprehensive studies on measurements and modeling of species mole fraction profiles for low-pressure premixed DME flames with equivalence ratios ranging from near-stoichiometric conditions to fuel-rich flames near the limits of flat flame stability using PI-MBMS and electron-ionization (EI) MBMS. They also investigated the isomer-specific influences on the composition of reaction intermediates in DME/propene and ethanol/propene mixture flames with particular emphasis on the formation of harmful emissions [5]. Xu et al. [6] used PI-MBMS to detect new intermediates and to measure mole fractions in the low-pressure laminar premixed stoichiometric ratio DME/O₂/Ar and ethanol/O₂/Ar flames, and five detailed oxidation mechanisms were used for the modeling study and a new one was proposed. Very recently, flame structures of CO₂-diluted DME flames at low-pressures were measured experimentally using

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Table 1 – Flame conditions for DME/H₂ flames at 40 mbar with equivalence ratios of 1.5. (Unit for reactants is mole fractions).

No.	R _{H₂} (%)	DME	H ₂	F–H ₂	O ₂	F–O ₂	Ar
1	0	0.2	/	/	0.4	/	0.4
2	20	0.184600	0.046200	/	0.384600	/	0.384600
3	20	0.184600	/	0.046200	0.369200	0.015400	0.384600
4	40	0.163636	0.109091	/	0.363636	/	0.363636
5	40	0.163636	/	0.109091	0.327272	0.036364	0.363636

EI-MBMS and also high-pressure flame speeds of lean and rich DME flames with and without CO₂ dilution were measured in a nearly-constant-pressure vessel [7].

Hydrogen is also extensively studied as a clean fuel or fuel additives due to its high flame speed, wide flammability range, low ignition energy and low emissions etc [8,9]. Chen et al. [8] experimentally measured the combustion intermediates of DME/H₂ blended fuel flames. Liu et al. [9] numerically studied the effects of H₂ addition on DME flames. When H₂ is added into fuel, the DME mole fraction is decreased and then the features of combustion could be changed accordingly including mole fractions of major species and intermediate species etc. However, we don't know that these changes are due to dilution and thermal effects of H₂, or because of the chemical reactions of H₂. Until now, to our best knowledge, there is little work on this topic concerning the detailed effects of the reactive additive H₂ in the fuel mixture DME/H₂ flame. The present study is devoted to obtain the actual chemical effects of H₂ addition on DME flames by numerical kinetic analysis.

Kinetic modeling and analysis method

The detailed chemical mechanism for DME oxidation and combustion developed by Zhao et al. [10] was used here. The mechanism consists of 56 species and 290 reactions, and was validated against high- as well as low-temperature flow reactor and jet-stirred reactor data, shock tube ignition delays, and laminar flame species as well as flame speed measurements [10]. Moreover, the H₂ oxidation sub-mechanism developed by Li et al. [11] was included in this mechanism. Model predictions for freely propagated premixed laminar low-pressure DME/H₂ flames are obtained using a modified ChemkinII/Premix code [12] and the calculations include multi-component molecular diffusion and thermal diffusion. The calculations domain was from –2.0 cm at the upstream to 10.0 cm at the downstream for sufficiently long to achieve the adiabatic equilibrium at the downstream. The upstream initial temperature is set to 300 K and pressure is 40 mbar. Here it is more convenient to use low-pressure rich flames due to better resolutions of the thicker flat flames and available experimental devices [3–8]. We focus on the variations of mole fractions of different species and the burning velocity discussion is beyond the scope of this study. The equivalence ratios for all the flame are the same with 1.5. The flame conditions are shown in Table 1. The oxidizer in the present flames is oxygen. Here the temperatures are obtained by solving energy equations. The original flame conditions were taken or calculated from Refs. [8,9]. The added hydrogen fraction (R_{H₂}) is defined as the mole fraction of H₂ in the DME/H₂ fuel blends.

It was pointed out by Du et al. [13] that three categories of effects of additives are potentially important: (a) dilution effect due to reduction in the concentrations of the reactive species and their collision frequencies, (b) thermal effect due to the change in flame temperature, and (c) direct chemical effect because of the participation of the additives in the chemical reactions. Moreover, Liu et al. [14] clarified that the variation of the flame temperature caused by the direct participation of an additive in chemical reactions should be considered as part of the chemical effects of the additive rather than its thermal effect.

The following analysis method was proposed for analyzing the chemical effects of H₂ addition on the DME/H₂ blended fuel flame based on the modification from the analysis method in Refs. [7,14]. In the present study the added H₂ is assumed as normal H₂ and fictitious or fake H₂ (written as F–H₂) to assess the real chemical effect of H₂. Normal H₂ is allowed to participate in chemical reactions in flames. Fictitious H₂ has exactly the same thermochemical, transport data and the same third-body collision efficiency as the normal H₂ but is not allowed to participate in all related chemical reactions in flames. More importantly in the present analysis, to keep the same equivalence ratios for all the flame conditions including those conditions with fictitious H₂ addition, from the point of view of the numerical analysis, a part of oxygen should be separated as fictitious O₂ (written as F–O₂) from total O₂. Similarly with F–H₂, the fictitious O₂ has exactly the same thermochemical, transport data and the same third-body collision efficiency as the normal O₂ but is not allowed to participate in all related chemical reactions in flames.

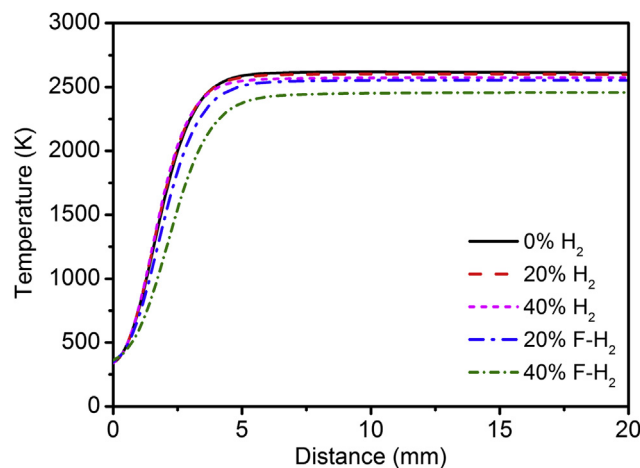


Fig. 1 – Temperature profiles of DME/H₂ flames with different levels of hydrogen addition.

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