Research article

Study on effect of dimethyl ether addition on combustion characteristics of turbulent methane/air jet diffusion flame

Yinhu Kang [a,b,*], Wei Shuang [c], Xingchi Jiang [b], Yangfan Song [d], Sicong Sun [d], Pengyuan Zhang [b], Yuming Sun [b], Xiaofeng Lu [d], Quanhai Wang [d], Xiaolong Gou [d], Xuanyu Ji [e]

[a] Postdoctoral Station of Environmental Science and Engineering, Chongqing University, Chongqing 400045, China
[b] Key Laboratory of the Three Gorges Reservoir Region's Eco-Environment, Ministry of Education, Chongqing University, Chongqing 400045, China
[c] Sichuan Electric Power Design & Consulting Cor. LTD, Chengdu 610041, China
[d] Key Laboratory of Low-grade Energy Utilization Technologies and Systems, Chongqing University, Ministry of Education of China, Chongqing 400044, China
[e] College of Mechanical and Power Engineering, Chongqing University of Science & Technology, Chongqing 401331, China

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ABSTRACT

The kinetics and soot and NOx emission characteristics of the CH_4/dimethyl ether (DME) jet diffusion flames (JDFs) are studied by experiments and simulations with a detailed chemical mechanism. The results showed that decomposition of DME in the pyrolysis zone generated massive CH_3, which changed the local flame structure and soot-correlated chemistry to some extent. Due to reductions of the incipient species concentrations including benzene (A1), pyrene (A4), C_3H_3, and C_2H_2, soot loading of the CH_4 JDF decreased by reducing margins with DME addition. A1 and thus soot formation rates due to DME addition were most sensitive to the recombination reaction of C_3H_3 ($C_3H_3 + C_3H_3 = A1$). With respect to the CH_4/DME JDFs, NOx was emitted mainly through the thermal and prompt pathways. The thermally-generated EI_{NOx} increased exponentially with DME addition because of the increasing enhancement of OH concentration in the radical pool. By contrast, the promptly-generated EI_{NOx} decreased in reducing margins with DME addition because of the reducing decrease in CH concentration. The synergistic effect of DME addition on the total NOx emission, i.e. the overall EI_{NOx} decreased firstly and then increased with DME addition, was examined in this paper. Additionally, it is reported that the 40%CH_4/60%DME case was comprehensively optimal in terms of soot and NOx emission reductions.

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1. Introduction

Fossil fuels as well as its utilization and processing patterns are significantly crucial to the human civilization, since the power generation, manufacturing, and transportation industries rely highly on its combustion process. With the large reserve on the planet and its clean-combustion property, natural gas (NG) is applied to various combustion and engine systems, and research into its combustion characteristics has been extensively investigated in the scientific community [1].

Currently, several weaknesses associated with NG combustion are still obvious, which threats its application considerably. For instance, being the simplest and shortest alkane, methane (the major component of NG) is featured with the highest ignition temperature among all of the alkane candidates, which is responsible for the difficulty of ignition of the NG-fuelled engines. Secondly, although the NG jet diffusion flame (JDF) supplies the smallest carbon input given equal volumetric fuel flow rate, it usually emits much more soot versus the traditional hydrocarbons, like liquefied petroleum gas (LPG) [2].

By far, extensive fundamental research has been reported in the literature to conquer these weaknesses. One of the most efficient methods is to develop the dual fuel blends, by adding a fraction of oxygenated fuel to the target hydrocarbons.

Dimethyl ether (DME, CH_3OCH_3) has been regarded as a promising surrogate fuel in the past few decades. As the simplest ether without any C—C bonds in its molecular structure, DME has the lowest C/H ratio after methane, and its physical properties are rather similar with those of LPG [3].

Because of the excellent atomization and ignition properties of the liquid DME, fairly low emissions of soot particles, unburned hydrocarbons (HC), CO, and acoustic noise generation were reported previously [3–12]. It is well accepted that DME was very suitable to the compression-ignition (CI) engines as a neat fuel or fuel additive. This was not only due to its lower auto-ignition temperature and instantaneous vaporization after injection into the cylinder, but also due to the higher oxygen content (35 wt%) and absence of C—C bonds in its molecular structure. Currently, DME is generally utilized as a fuel additive to enhance the ignition, combustion, and emission performances of the

* Corresponding author at: Postdoctoral Station of Environmental Science and Engineering, Chongqing University, Chongqing 400045, China.
E-mail address: cqukangyh@cqu.edu.cn (Y. Kang).

traditional fuels, and many studies have been made to investigate the effect of DME addition on the combustion characteristics of diesel [13–15] or n-butane [16,17] under the engine combustion conditions. It was well verified by experiments that just a small fraction of DME addition could significantly reduce the ignition delay time [13] and emission indices of particulate matter (PM), HC, and CO [14,15] of diesel. In addition, DME has also been applied to the industrial boiler [18–23] and gas turbine [24–26] more recently.

Apart from the diesel/DME blends, DME was also mixed with the gaseous hydrocarbons such as methane to improve their combustion performance. The effect of DME addition on methane combustion characteristics were extensively studied in the literature. Burke et al. [27] developed a detailed chemical kinetic mechanism for the methane/DME mixture, which was capable of reproducing the ignition delay time in a wide range of operational parameters for the CI engines and gas turbines ($T = 600$–1600 K, $p = 7$–41 atm, and equivalence ratio = 0.3–2.0). Additionally, accuracy of this mechanism was also verified by comparison with the experimental data of flow reactor, jet-stirred reactor, shock-tube ignition delay time, shock-tube speciation, and laminar flame speed. By experiments on shock tubes and a rapid compression machine, as well as simulations using this chemical mechanism, the chemical kinetic behavior associated with ignition delay of the methane/DME mixture at high pressures was clarified.

Dai et al. [28] made numerical simulations with detailed chemistry and transportation models to study the kinetic and transportation effects involved in methane ignition enhancement due to H_2 or DME addition. It was reported that with regard to the homogeneous ignition, DME addition was more effective versus H_2 to improve the ignition of CH_4/air premixture. With respect to the non-premixed ignition process, H_2 addition was shown to be always more effective than DME. Additionally, the chemical kinetics and reaction pathways associated with the ignition enhancement of H_2- or DME-methane binary fuel mixture were also clarified.

The dual-fuel combustion regime in CI engines is usually made up of a small pilot injection of high-cetane fuel (like biodiesel) which ignites a premixture of high-octane fuel (like methane) with air. Namasivayam et al. [29] made measurements to compare the effects of biodiesel, emulsified biodiesel (biodiesel mixed with varying concentrations of water), and dimethyl ether as the pilot fuel on combustion behavior of the NG-fuelled engines, in terms of smog, NOx, HC, and CO emissions, and engine thermal efficiency. It was found that the emulsions performed very poorly as the pilot fuel, since they would enhance HC and CO emissions compared with the neat biodiesel pilot case. With regard to the DME pilot case, HC and CO emissions were lower than the emulsion case. In addition, the NOx emission and engine thermal efficiency were also maintained at lower levels in the DME pilot case. Hence, DME was a more efficient pilot fuel to enhance the NG engine performance.

Lowry et al. [30] investigated the laminar flame speed, Markstein length, and Lewis number of the methane/DME blends with varying blending ratios, over a wide range of initial pressures ranging from 1 to 10 atm. The experiments indicated that for the 80%methane/20%DME blends, the flames remained stable throughout the entire pressure range, which was ascribed to that the Lewis number kept near unity with the increment in equivalence ratio. However all other pure fuels and blends exhibited flame instability as the initial pressure was equal or higher than 5 atm, which was due to decrease of the Lewis number as the equivalence ratio increased. In addition, a small amount of DME addition could lead to a large change in the Markstein length. Yu et al. [31] studied the laminar flame speed, Markstein length, and stability of the methane/DME/air premixed spherical flames at different initial temperatures (303–453 K), pressures (1–7 atm), dilution ratios (0–25%), equivalence ratios (0.7–1.6), and a wide range of blending ratios (from pure methane to pure DME). It was reported that with the increment in DME addition, the laminar flame speed as well as intrinsic hydrodynamic instability was enhanced, and the sensitivity coefficient of pressure decreased.

Yoon et al. [32] studied the polycyclic aromatic hydrocarbon (PAH) and soot formation behaviors of the counterflow diffusion flames of methane, ethane, propane, and ethylene fuels blended with varying DME additions, using the planar laser-induced incandescence and fluorescence techniques. It was found that DME addition could reduce PAH and soot concentrations of the methane, ethane, and propane flames. However PAH and soot volume fractions in the ethylene/DME flame were enhanced versus the pure ethylene flame. Simulations with a detailed chemical mechanism showed that in the low-temperature region of the ethylene/DME flame where PAH grows, DME was decomposed to massive methyl radicals, which could increase propargyl concentration and enhance the incipient benzene ring formation through the propargyl recombination reaction. As a result, PAH and soot formations were enhanced with DME addition.

Roy et al. [33] made a numerical study to address the impacts of airstream dilution and jet velocity on NO emission characteristics of CH_4 and DME bluff-body flames. It was reported that airstream dilution by both CO_2 and H_2O could reduce the NO emission for both of the fuels. The effectiveness of H_2O dilution in NO emission reduction was more prominent. Additionally, for the same amount of diluents, the global NO reduction of the DME flame was higher in comparison with that of the methane flame.

Gabet et al. [34] compared the structure of turbulent DME and methane jet flames using the laser-based imaging techniques (CH_2O PLIF and Mie scattering). The CH_2O PLIF signals of the turbulent DME flame were nearly two orders of magnitude higher than that of the methane flame. Rankin et al. [35] compared fluid dynamics of the turbulent DME and methane non-premixed and partially-premixed flames, based on radiation intensity imaging measurements. It was found that the peak radiation intensity of the non-premixed and partially-premixed DME flames were approximately 15% and 30% larger in comparison with the corresponding methane flames. Additionally, Fuest et al. [36] employed the simultaneous 1-D Raman/Rayleigh scattering and LIF techniques to measure the instantaneous species concentration and temperature scalar profiles in two turbulent piloted, partially-premixed DME/air jet flames. Comparisons of the DME flames with the well-known Sydney/Sandia piloted methane jet flame series (A-F) showed that the finite-rate chemistry effects such as local extinction and re-ignition as well as their impacts on the scalar flame structure were quite different in the DME flames as compared to the methane flames.

In addition, Zhang et al. [37] systematically investigated the effect of DME addition on explosion behavior of the methane/air premixture, in terms of flammability limits, maximum explosion pressure, and maximum rate of pressure rise.

Since the JDF is an ideal model of many practical combustion systems such as internal combustion engines, gas turbines, and boiler, etc., studies on the combustion characteristics of methane/DME JDF are particularly valuable for the industrial application. In the present study, experiments and simulations were conducted to investigate the effect of DME addition on the combustion characteristics of the methane/air coaxial JDF, in terms of flame structure and soot and NOx emissions, which would be useful for optimization design and operation of the practical DME/NG-fuelled combustion systems.

2. Experimental section

2.1. Experimental apparatus

The experimental apparatus with the measuring system, as schematically shown in Fig. 1, was described in details in our previous study [22]. Hence it is just presented briefly herein. As Fig. 1 shows, a co-axial jet burner, consisting of an inner fuel nozzle (internal diameter 3.00 mm, external diameter 8.00 mm) and an outer annular coflow tube (internal diameter 100 mm, external diameter 108 mm), was employed for the experiments. A glass bead layer (100 mm in thickness) and a honeycomb screen (50 mm in thickness) were installed