Available online at www.sciencedirect.com

Combustion and Flame 154 (2008) 368–377

Combustion and Flame

www.elsevier.com/locate/combustflame

Synergistic effect of mixing dimethyl ether with methane, ethane, propane, and ethylene fuels on polycyclic aromatic hydrocarbon and soot formation

S.S. Yoon [a], D.H. Anh [b], S.H. Chung [c,*]

[a] Corporate Research & Development Division, Hyundai-Kia Motors, Gyeonggi-do 445-706, Republic of Korea
[b] Korea Electric Power Research Institute, Daejeon 305-380, Republic of Korea
[c] School of Mechanical and Aerospace Engineering, Seoul National University, Seoul 151-742, Republic of Korea

Received 1 August 2007; received in revised form 24 January 2008; accepted 7 April 2008

Available online 26 May 2008

Abstract

Characteristics of polycyclic aromatic hydrocarbon (PAH) and soot formation in counterflow diffusion flames of methane, ethane, propane, and ethylene fuels mixed with dimethyl ether (DME) have been investigated. Planar laser-induced incandescence and fluorescence techniques were employed to measure relative soot volume fractions and PAH concentrations, respectively. Results showed that even though DME is known to be a clean fuel in terms of soot formation, DME mixture with ethylene fuel increases PAH and soot formation significantly as compared to the pure ethylene case, while the mixture of DME with methane, ethane, and propane decreases PAH and soot formation. Numerical calculations adopting a detailed kinetics showed that DME can be decomposed to produce a relatively large number of methyl radicals in the low-temperature region where PAH forms and grows; thus the mixture of DME with ethylene increases CH_3 radicals significantly in the PAH formation region. Considering that the increase in the concentration of O radicals is minimal in the PAH formation region with DME mixture, the enhancement of PAH and soot formation in the mixture flames of DME and ethylene can be explained based on the role of methyl radicals in PAH and soot formation. Methyl radicals can increase the concentration of propargyls, which could enhance incipient benzene ring formation through the propargyl recombination reaction and subsequent PAH growth. Thus, the result substantiates the importance of methyl radicals in PAH and soot formation, especially in the PAH formation region of diffusion flames.

© 2008 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

Keywords: Soot; Polycyclic aromatic hydrocarbon (PAH); Dimethyl ether (DME); Counterflow diffusion flame; Synergistic effect; PAH growth

1. Introduction

Soot formation is a complex process involving the pyrolysis of fuel, the formation and growth of aromatic hydrocarbons and soot particles, and the oxidation of soot. Hydrocarbon species generated from fuel

---

* Corresponding author. Fax: +82 2 883 0179.
E-mail address: shchung@snu.ac.kr (S.H. Chung).

0010-2180/$ – see front matter © 2008 The Combustion Institute. Published by Elsevier Inc. All rights reserved.
doi:10.1016/j.combustflame.2008.04.019

pyrolysis lead to incipient ring formation such as benzene (C_6H_6) and naphthalene ($C_{10}H_8$), which grow to polycyclic aromatic hydrocarbons (PAHs) and finally to soot [1–3]. The role of acetylene (C_2H_2) species, which maintain a high concentration in the soot formation region due to their chemically stable structure, has been emphasized throughout the overall soot formation process by the H-abstraction-C_2H_2-addition (HACA) mechanism [4–7].

Early models based on the HACA mechanism, however, sometimes underestimated the PAH and soot formation [8,9]. Alternatively, odd-carbon chemistries related to resonantly stable radicals, such as propargyl (C_3H_3), cyclopentadienyl (C_5H_5), and benzyl (C_7H_7), have been introduced to refine the formation rates of PAH and soot. The propargyl recombination reaction has been suggested as one of the dominant pathways for benzene formation [10–12] and the role of odd carbon chemistries related to propargyl radicals has been emphasized for PAH growth [13–15].

It has been recently reported that the diffusion flames of mixture fuels of ethylene and propane (or ethane) enhances the formation of PAHs and soot considerably as compared to those with the respective fuels [15–18]. This synergistic effect, defined as the case when a mixture fuel can produce more PAH and soot as compared to the respective pure fuels, has been explained based on the role of methyl radicals, which are supplied by the decomposition reactions of carbon bonds in ethane and propane, since methyl radicals can increase the formation of propargyl (C_3H_3) radicals through the reaction $pC_3H_4 + CH_3 = C_3H_3 + CH_4$ in the PAH formation region [18]. Subsequently, odd carbon chemistries involving propargyl could enhance the benzene formation and also the PAH growth for the mixture fuels. Together with the importance of the HACA reaction, the synergistic effect arises.

The synergistic effect on soot formation has also been observed when methane or air is added to the ethylene fuel [19–23]. This has also been explained based on the role of methyl radicals through the reactions $CH_4 + H = CH_3 + H_2$ and $C_2H_4 + O = CH_3 + CHO$, respectively. The results again emphasized the importance of odd-carbon-atom chemistries, since the propargyl formation was enhanced by the reactions of $C_1 + C_2$.

Recently, oxygenated fuels have received considerable attention as alternative fuels in reducing the emission of particulate matter (PM) from practical combustors such as diesel engines [24–28]. Dimethyl ether (DME, CH_3–O–CH_3), which has two methyls with an oxygen atom in its fuel structure, has been suggested as a promising fuel for diesel engines because of low PM emission characteristics. Song et al. [26] have shown that oxygenated fuels can be soot removers when they are mixed in diesel fuel, having an appreciable soot reduction tendency. The mixing of DME with hydrocarbon fuels has also been investigated with regard to their low-temperature autoignition characteristics in homogeneous-charge compression ignition (HCCI) engine development. Konno and Chen [27] and Morsy and Chung [28] demonstrated that DME can be a viable ignition improver when mixed with hydrocarbon fuels.

Even though pure DME fuel is known as a clean fuel in terms of soot formation, the methyl groups together with oxygen contained in the DME fuel structure could play an important role in the formation of PAHs and soot when DME is mixed with other fuels. Methyl and oxygen radicals can be generated through the decomposition of DME in the initial pyrolysis process. Considering the role of methyl and oxygen radicals in the formation of PAHs and soot, mixture of DME with various hydrocarbon fuels would exhibit an enhancing effect on PAH and soot formation. Recently, the mixing of oxygenates, such as DME and ethanol (C_2H_5OH), in ethylene fuel has been tested experimentally and numerically in coflow diffusion flames [29,30], exhibiting a synergistic effect on soot formation. McEnally and Pfefferle [29] showed that the oxygenates decompose to methyl radicals, which enhance the rate of formation of propargyl radicals through the reactions of $C_1 + C_2$; thus the synergistic effect can be explained based on odd carbon atom pathways such as benzene formation from self-recombination reaction of propargyl radicals. McNesby et al. [30] indicated that the methyl radicals from the ethanol enhanced the rate of benzene formation through the even carbon pathways of $CH_3 + C_3H_3 = C_4H_6$ and $C_4H_5 + C_2H_2 = C_6H_6 + H$.

The present work is a complementary study of DME mixing with hydrocarbon fuels in a counterflow configuration. An experiment and numerical simulations have been performed to further elucidate the effect of DME on PAH and soot formation. DME was mixed with the hydrocarbon fuels of methane, ethane, propane, and ethylene, and corresponding PAH and soot concentrations were measured by adopting laser-induced fluorescence (LIF) and laser-induced incandescence (LII) techniques, respectively. To confirm the roles of CH_3 and C_3H_3, pyrolysis paths from the respective fuels to CH_3, C_2H_2, C_3H_3, and O radicals were simulated using a detailed kinetic model.

2. Experiment and numerical calculation

The experimental apparatus consisted of a counterflow burner, a flow control system, and laser diagnostic setups. The counterflow burner consisted

Download English Version:

https://daneshyari.com/en/article/167823

Download Persian Version:

https://daneshyari.com/article/167823

Daneshyari.com