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Chemical kinetic effect of hydrogen addition on ethylene jet flames in a hot and diluted coflow



F. Wang^{a,*}, P. Li^b, J. Mi^b, J. Wang^a, M. Xu^c

^a Department of Building Environment & Energy Engineering, School of Environmental Science & Engineering, Huazhong University of Science & Technology, Wuhan 430074, China

^b State Key Laboratory of Turbulence & Complex Systems, College of Engineering, Peking University, Beijing 100871, China

^c Marine Engineering College, Dalian Maritime University, Dalian 116026, China

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ABSTRACT

This paper numerically investigated the chemical kinetic effect of hydrogen addition, ranging from 0% to 60% (by vol.), on ethylene jet flames in a hot coflow. The Eddy Dissipation Concept model with the San Diego mechanism was used for all the calculations. To validate the present modeling, four flames were predicted under the experimental conditions of Medwell et al. [Combust. Flame 152 (2008) 100–113] and the predictions are found to agree quite well with the measurements. As the hydrogen content is higher, the jet entrainment and the jet velocity decay are enhanced, whilst the local equivalence ratio in the reaction zone is decreased. Moreover, under MILD condition, the hydrogen addition leads to remarkable increases in the mole fractions of H, O and OH radicals in the reaction zone, which then promotes the oxidation of C₂H₄ significantly. When hydrogen is added, the increasing rate of H mole fraction is greater than that of OH mole fraction. This hence makes the reactions attacked by H strengthened while those attacked by OH weakened. With respect to those at traditional air condition, the higher-carbon path (C₂H₄ → C₂H₃ → C₂H₂ → C₂H, HCCO → CH₂CO → CO → CO₂) of the C₂H₄ oxidation at MILD condition becomes more important while the lower-carbon path (C₂H₄ → [C₂H₅ →] CH₃ → [S-CH₂, T-CH₂, CH₃O, CH₃OH, and CH₂OH] → CH₂O → HCO → CO → CO₂ and C₂H₄ → [C₂H₅ →] CH₃ → [S-CH₂ → T-CH₂] → CO → CO₂) is weakened. Further, under MILD condition at X_{O₂}^{*} = 3%, the H₂ addition weakens the importance of higher-carbon path but enhances that of the lower-carbon path, thus the C₂H₂ mole fraction is greatly reduced. Considering that C₂H₂ is an important precursor of soot, the decrease of C₂H₂ mole fraction and the local equivalence ratio indicate that H₂ might have the potential to reduce the soot emission.

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* Corresponding author. Tel.: +86 132 9416 0016.

E-mail address: ffwang@hust.edu.cn (F. Wang).

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Introduction

MILD (moderate or intense low-oxygen dilution) combustion [1] has been recently recognized as a promising technology, due to its potential in enhancing thermal efficiency and simultaneously reducing NO_x emissions. This combustion, rigorously defined by Cavaliere and Joannon [1], can be realized by mixing air and/or fuel with combustion products, so that the combustible mixture has a temperature above its auto-ignition temperature (T_{si}). Therefore, the diluted and preheated mixture can be ignited spontaneously, while the temperature rise during combustion is lower than the corresponding T_{si} . Although not identical [2], MILD combustion [1], HiTAC (high temperature air combustion) [3], FLOX (flameless combustion/oxidation) [4], and CDC (colorless distributed combustion) [5] may be classified into the same type of combustion technology.

To explore a wider application of MILD combustion, it is of great interest to fundamentally understand this interesting technology. To achieve MILD combustion, the reactants are typically diluted and preheated by the hot flue gases, either externally or internally, so that the combustion feature, such as the stabilization mechanism, the structure of the reaction zone, and the ignition, might be varied greatly. Although some attempts on the MILD combustion were conducted in practical furnaces [3–9], fundamental studies are short [1,2], due to the complex environment inside such enclosed systems. Instead, to mimic the effect of the dilution and preheating caused by the intense recirculation during MILD combustion, a jet flame into hot coflow (JHC) is developed [10], using which the combustion parameters can be studied independently and decoupled from the integration of the complex flow and chemical kinetics.

Owing to its advantages in the simplicity and controllability, the JHC burner system has been widely utilized for experiments in investigating MILD combustion by the research institutes all over the world [10–34], as summarized in Table 1. Dally et al. [10] used then advanced laser diagnostics techniques to investigate the flame structure of CH_4/H_2 JHC flames and deduced that a different mechanism of CO and NO formation might exist under MILD condition. This work was then extended by Medwell et al. [11–14], where the dependence of the flame stability and the lift-off height on the fuel/coflow composition and the distributions of the OH radical and the formaldehyde intermediate were provided. Sepman et al. [15–18] reported the spatial structure and NO formation of a laminar CH_4/N_2 JHC flames under MILD conditions. These authors found that the NO formation in the MILD combustion appears to be negligible (few ppm), most of which results from the prompt-NO. Oldenhof et al. [19–22] studied the effect of the flow field on the JHC flames and confirmed its importance on the stabilization of the JHC flames. Also the effects of hydrogen addition on the reaction zone structure of the JHC flames were reported [17,23]. Moreover, Choi et al. [30–33] observed that a decrease in the lift-off height of the CH_4/N_2 or n-heptane JHC flames with increasing the jet velocity under MILD condition, similar to that measured by Medwell et al. [11,14]. Such a behavior of the lift-off height is inconsistent with the trend reported in the traditional lifted jet flame and

was deduced to be the results of the premixing of the fuel jet and oxygen before any reaction takes place [35].

In addition to the experimental work, the modeling of JHC flames has also attracted good attention to either replicating the measurements [36–39] or understanding the physical/chemical observations [40–46]. For the first issue, Christo and Dally [36] found that the utilization of the EDC model with GRI-Mech 3.0 can satisfactorily predict the flow and combustion characteristics of the JHC flames. Mardani et al. [37] found that the molecular diffusion is important in modeling the JHC flames, especially under MILD conditions. Aminian et al. [38] discussed the applicability of the EDC model in predicting the JHC flames under MILD condition and found that a modification in the fine structure residence time constant can predict the temperature and major combustion products more accurately when the local turbulence Reynolds number is greater than 65. Following this, Shabaniyan et al. [39] found that the predicted results using the modified EDC model as well as the PDF transport model both agree well with the measurements of the C_2H_4 jet flames (either undiluted or diluted with H_2 , air or N_2). On the other aspect, Mardani et al. [40] found that the reaction rate of the CH_4 JHC flame increase gradually with hydrogen addition, as concluded also in other studies [17,41,42]. Moreover, Mei et al. [43] systematically summarized the dependence of the dimension of a CH_4 jet flame on the oxygen content, velocity and temperature of the hot O_2/CO_2 coflow. In addition, for the CH_4/H_2 flames under MILD condition, the chemical path including the conversion of methyl (CH_3) to higher hydrocarbons is activated in forming CO and CO_2 [44] and the NNH and prompt routes are the main source of NO formation [45].

According to the above discussion and Table 1, most studies on the JHC flames are mainly focused on the fuel of CH_4 or H_2 , or both, due to their relative simple chemical structure. On the contrary, the present work is to study the $\text{C}_2\text{H}_4/\text{H}_2$ JHC flames, which might advance our knowledge from the combustion of the simple fuel (e.g., CH_4) to that of other practical fuels with complex chemistry. After validating the modeling by the measurements of Medwell et al. [11], this study investigates the chemical kinetic effect of hydrogen addition on the C_2H_4 jet flames. More specially, the variations of the flow and temperature field, reaction structure (e.g., the distributions of the species and its producing/consuming rate) are presented for the flames with different hydrogen content. Also, the main paths for the oxidation of the C_2H_4 JHC flames, with and without hydrogen addition, are compared quantitatively.

Description of the burner and modeling

Configuration of the JHC burner system

The present simulated JHC burner system is similar to that used by Medwell et al. [11] and a brief description of the system is given here. In their experiments [11], the system consisted of an insulated and cooled central fuel jet (i.d. = 4.6 mm), which was surrounded coaxially by an annulus nozzle (i.d. = 82 mm). A premixed secondary burner, mounted upstream of the jet exit plane, was used to provide hot

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