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Flame attachment and kinetics studies of laminar coflow CO/H_2 diffusion flames burning in O_2/H_2O

Huanhuan Xu[a,b], Fengshan Liu[b], Shaozeng Sun[a,*], Yijun Zhao[a], Shun Meng[c], Lei Chen[a], Longfei Chen[d,*]

[a] Combustion Engineering Research Institute, School of Energy Science and Engineering, Harbin Institute of Technology, PR China
[b] Measurement Science and Standards, National Research Council Canada, Building M-9, 1200 Montreal Road, Ottawa, ON K1A 0R6, Canada
[c] School of Automotive and Transportation Engineering, Hefei University of Technology, Hefei, PR China
[d] School of Energy and Power Engineering, Beihang University, 37th Xueyuan Road, Haidian District, Beijing 100191, PR China

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ABSTRACT

In this study, experimental and numerical investigations were conducted to study the attachment and oxidation process of laminar CO/H_2 diffusion flames burning in coflow O_2/H_2O at 1 atm with an inlet temperature of 400 K for both the fuel and oxidizer streams. The effects of fuel composition were investigated by considering a wide range of CO/H_2 mole ratio from 95%CO–5%H_2 to 5%CO–95%H_2 and also pure H_2. The oxidizer has a fixed composition of 75%H_2O–25%O_2. The measured flame heights determined by OH^*-chemiluminescence images were used to validate the flame model adopted in this work. Through numerical simulations using a two-dimensional flame code with the preheating effect, detailed reaction mechanism, and detailed thermal and transport properties, the details of flame attachment and flame structure were obtained and analysed. Although both CO and H_2 diffuse over the burner rim and move upstream into the oxidizer stream, the attachment point of a H_2-rich syngas flame is further upstream below the burner exit than that of a CO-rich flame. This is attributed to the high reactivity of H_2 through reaction $OH + H_2 = H + H_2O$ and the high diffusivity of H_2. Reaction pathways for syngas burning in the oxidizer of O_2/H_2O based on a detailed kinetics analysis were revealed, not only inside the fuel tube and above the fuel exit, but also near the flame sheet and in the flame attachment zone. Significant consumption of H_2O was observed in the flame core due to the reverse reaction of $OH + H_2 = H + H_2O$ which shifts to proceed forward outside the flame in the radial direction also at higher streamwise locations if H_2 in the fuel flow is rich, oxidizing unburned H_2 to H_2O.

1. Introduction

The desire to achieve high energy conversion efficiency and zero pollutant emissions has fostered a strong interest in the oxy-fuel combustion technology. This technology can accommodate different types of fuel, varying from natural gas [1], pulverized coal [2] to syngas [3], and the combustion products of a hydrocarbon fuel consist mainly of H_2O and CO_2, resulting in the merit of easy capture and storage of CO_2 by simply condensing the steam in the flue gas. During the research and development of oxy-fuel combustion technology, various cycle concepts using CO_2 or H_2O as the recycle working fluid have been proposed, such as the MATIANT cycle [4], the Graz cycle [5], and the water cycle [6] developed by Clean Energy Systems (CES), Inc. In particular, some studies have demonstrated the advantages of steam/water oxy-fuel combustion (H_2O as the recycle fluid) with good combustion stability [7], low investment, high efficiency, and zero pollutant emissions [8,9].

It is anticipated that the steam/water oxy-fuel combustion behaviour will be significantly different from the conventional air-fuel combustion due to the substitution of water vapour for nitrogen as diluent in the oxidizer stream. Firstly, H_2O will affect the chemical reaction by participating in some elementary reactions and can also affect the combustion process though a very strong third-body collision efficiency, which has been shown by Seiser et al. [10]. Secondly, H_2O has a lighter molecular weight than N_2, which enables a higher diffusivity. Thirdly, the high specific heat and radiative property of H_2O also plays important roles in influencing the combustion process through moderating the temperature. Numerous studies have been conducted to study the thermodynamics [11,12], economic performance [13–15], and pollutant reduction efficiency [8] of steam/water oxy-fuel combustion systems. However, less attention has been paid to the combustion

* Corresponding authors.
E-mail addresses: sunsz@hit.edu.cn (S. Sun), chenlongfei@buaa.edu.cn (L. Chen).

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characteristics, especially the flame structure and the oxidation process in such unusual combustion systems, which are expected to directly depend on the fuel and oxidizer compositions. This fundamental knowledge is particularly important to understand the combustion behaviour and critical to optimize the combustor design of steam/water oxy-fuel combustion systems.

As a promising alternative fuel, syngas has been of great interest for its extensive sources of feedstock and pollution-free potential. The main combustible components in syngas are CO and H_2. The physical and chemical properties of syngas differ greatly from those of the traditional hydrocarbon fuels, such as methane and propane, and modify the combustion process through the enhanced diffusion, intensified reactivity, and increased flame temperature as a result of the presence of H_2 [16,17]. On one hand, the existing experimental and numerical investigations conducted in the past few decades have shown the importance of the effects of preferential diffusion of H_2 and H on the flame temperature [18,19], OH distribution [20], and laminar burning velocity [20]. On the other hand, it is also well known that the reactivity of H_2 is much higher than that of hydrocarbon fuels, which enhances the laminar flame speed [16], extends the flammability [21], and favours the oxidation of methane [22]. In contrast, it has been reported [23] that when CO and methane are both supplied as reactants, the CO oxidation follows that of methane, indicating the lower reactivity of CO than that of CH_4. Since syngas composition varies significantly due to the different feedstocks and gasification techniques, research on the effect of syngas composition is one of the most concerned subjects.

Among all the studies related to the effect of syngas composition, the global combustion properties including the laminar flame speed, ignition delay time, flame structure and flammable limits, have been the main focus. It has been shown that increasing the H_2 fraction enhances the laminar flame speed of CO/H_2/air mixtures with or without inert gas (such as CO_2 and N_2) dilution [24–26]. In particular, Sun et al. [27] confirmed the enhancing effect of H_2 on the laminar flame speed of syngas with the presence of a considerable amount of H_2O. This effect on the laminar flame speed can be attributed to the enhanced chemical reaction rates and molecular diffusivity when the concentration of H_2 is increased [28]. Krejci et al. [29] investigated the ignition delay time of hydrogen and syngas blends using a high-pressure shock tube and found that carbon monoxide increases the ignition delay time except at low temperatures and pressures higher than 12 atm where the ignition delay times are indistinguishable as the CO fraction increases. Fu et al. [30] found that the production of H and OH radicals is promoted as the H_2 fraction increases through numerical investigations on laminar one-dimensional premixed flames. The study of Shih et al. [21] showed that a higher H_2 percentage in syngas leads to a wider flammable range. Besides, Hwang et al. [31] found that the detachment stability limit of syngas jet flame increases with increasing hydrogen content in the fuel stream. It is apparent that most previous studies of syngas have focused on the global flame properties (such as laminar flame speed, ignition delay and the flame stability) or the structure of 1D counterflow flame. Although these studies provided valuable fundamental knowledge and experimental data to understand the syngas combustion characteristics, they do not offer the same level of details as laminar coflow diffusion flames as far as the flame structure and flame attachment are concerned, albeit counterflow and coflow diffusion flames can be linked through the flamelet concept. In addition, laminar coflow diffusion flames are more relevant to flames in practical combustion systems, which are almost always multidimensional and turbulent.

Flame attachment is an important branch of research in jet diffusion flame stabilization and is an essential part of the flame base structure. Several experimental and numerical attempts have been made to gain insights into the characteristics of flame attachment in jet diffusion flames of various fuels. Chen et al. [32] proposed that the hot zone connected to the reaction kernel through the formation of HO_2 layer stabilizes the micro-jet methane diffusion flame. Takahashi et al. [33] believed that the laminar coflow CH_4/air diffusion flame attaches to the burner as a result of the back diffusion of chain radicals and fuel fragments based on numerical investigations without considering the thermal interactions between the flame and solid fuel tube. Moreover, our recent work [34] showed that the efflux of CH_4 to the air side over the burner rim is responsible for the attachment of a laminar coflow CH_4/air diffusion flame outside the fuel tube by considering the conjugate heat transfer between the burner wall and the surrounding fluids. However, these existing studies were all conducted for jet diffusion flames of single-component fuels and the preferential diffusion effect of multi-component fuels, such as syngas, on the flame attachment is not yet well understood. Although Gao et al. [35] studied the flame base structure of micro-jet hydrogen/methane diffusion flames with different H_2/CH_4 ratios, the flames base in their work always occurs upstream the burner rim and only the radial gap between the burner wall and the stabilized flame kernel, as a result of local extinction, differs with varying the H_2/CH_4 ratio. Gao et al. attributed the variation of the radial location of the flame base to the HO_2 production reaction, $H + O_2 + M = HO_2 + M$, because this reaction plays a dominant role in sustaining the reactivity at the flame base. In summary, no studies have been reported in the open literature so far to investigate the effects of fuel composition on the attachment of syngas jet diffusion flames.

The oxidation process highly depends on chemical reactions and heat and mass transfer processes and directly affects the flame stabilization and structure as well as pollutant formation. Numerous investigations have been carried out to study the oxidation process in one dimensional premixed and diffusion flames [21,27]. However, there have been limited studies to investigate the detailed oxidation process in multidimensional syngas diffusion flames where the physical and chemical processes are intimately coupled in a more complex way. Hossain and Nakamura [36] numerically investigated micro hydrogen-air diffusion flames and pointed out that H_2 is not consumed by OH in the fuel tube and H is mainly produced above the burner exit through reaction $OH + O = H + O_2$ then quickly diffuses upstream towards the burner. The back diffusion of ambient air into the burner for a low Reynolds number jet flow promotes the oxidative reactions at the vicinity of the burner tip. Khan et al. [37] explored the structure and reaction zone of syngas diffusion flames burning in quiescent air, but the kinetics analysis with regard to the syngas oxidation was limited to the radial direction at an axial location of $z = d$ (d is the inner diameter of the burner exit). Based on detailed numerical analyses, Cheng et al. [38] summarized the key oxidation steps in a microjet methane diffusion flame with the aim to reveal its stabilization mechanism. Zhang et al. [39] studied the non-premixed hydrogen micro-jet flame with a focus on the thermal interaction between the flame and solid fuel tube and no kinetics analyses were performed to understand the hydrogen oxidation process. Nevertheless, the above studies all focused on jet diffusion flames burning in air. The oxidation process of laminar coflow syngas diffusion flames burning in O_2/H_2O have not been investigated.

The objective of the present research is to study the effects of syngas composition on the structure of laminar coflow syngas diffusion flames burning in O_2/H_2O, seeking for a better understanding of the flame attachment mechanism and the oxidation process of such much-less studied flames. Results discussed in this study consist of four main parts. Observation of the syngas flames with varying fuel compositions is firstly presented. Then the diffusion vectors of several species are examined to gain insights into the mechanism of syngas flame attachment and to investigate the