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Characteristics and mechanistic analysis of CO formation in MILD regime with simultaneously diluted and preheated oxidant and fuel

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HIGHLIGHTS

- The ROP of CO of R167, R166, R79 and R23 markedly decrease with increasing Kv and ϕ.
- The CO formation is controlled by the consumption reaction R99 in MILD combustion.
- The reaction R99 has been a direct reaction in MILD combustion.

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ABSTRACT

The innovative combustion modality of moderate or intense low-oxygen dilution (MILD) combustion has high combustion efficiency and low pollutant emissions. In this paper, the characteristics and mechanisms of CO formation in the MILD combustion regime were studied using opposed diffusion flame (OPPDIF) with simultaneously diluted and preheated oxidant and fuel. The GRI 3.0 mechanism was adopted to represent the chemical reactions. The effects of the entrainment ratio (Kv), the equivalence ratio (ϕ), and the inlet temperature (T_{in}) on CO formation were studied under three calculation conditions: (1) the range of Kv from 1 to 8 at T_{in} = 1300 K, (2) the range of ϕ from 0.6 to 1.6 at T_{in} = 1300 K, and (3) the range of T_{in} from 1000 to 1300 K at Kv = 3 and ϕ = 1. The results show that in the MILD combustion regime, increasing entrainment ratio and equivalence ratio can reduce the emission of CO. However, their effects become weak when entrainment ratio exceeds 6. From the threshold states to MILD combustion regime, the EICO sharply decreases with increasing entrainment ratio and equivalence. Increasing inlet temperature can gently enhance the emission of CO in MILD combustion regime.

The main differences of the mechanisms of CO formation between in MILD combustion regime and in threshold state are two: (1) in the threshold states, C_2H_2 makes contribution comparable with CH_3 to the CO formation in the threshold state; due to oxidative reforming process, the path from CH_3 to C_2H_2 ($CH_3 \rightarrow C_2H_6 \rightarrow C_2H_5 \rightarrow C_2H_4 \rightarrow C_2H_3 \rightarrow C_2H_2 \rightarrow CO$) is greatly weakened in MILD combustion regime, causing that the contribution of CH_3 is up to be comparable with HCCO and the contribution of C_2H_2 is down to the lowest; (2) in threshold states, the ROP of CO of the elementary reaction, $OH + CO \Longleftrightarrow H + CO_2$, changes from positive value to negative value due to the increase in [OH]/[H]; the direct reaction of this elementary reaction predominate in MILD combustion regime, because its direct reaction prefers the lower temperature compared to its reverse-direction reaction. According to the sensitivity analysis of CO formation, the CO formation is mainly controlled by the direct reaction of the elementary reaction, $OH + CO \Longleftrightarrow H + CO_2$, in the MILD combustion regime. The importance of the role of this elementary reaction increases with increasing the dilution and the equivalence ratio and decreases with increasing the inlet temperature.

1. Introduction

According to Cavaliere and de Joannon [1], in the moderate or intense low-oxygen dilution (MILD) combustion regime, the temperature of a reactant mixture should be above the auto-ignition temperature, and the oxygen concentration in the reactant mixture should be highly diluted with hot combustion products, typically to a concentration of no more than 3–5% [2]. As an innovative combustion modality, MILD combustion has a high combustion efficiency and low pollutant emissions and has therefore received increasing attention in recent decades [3–5].

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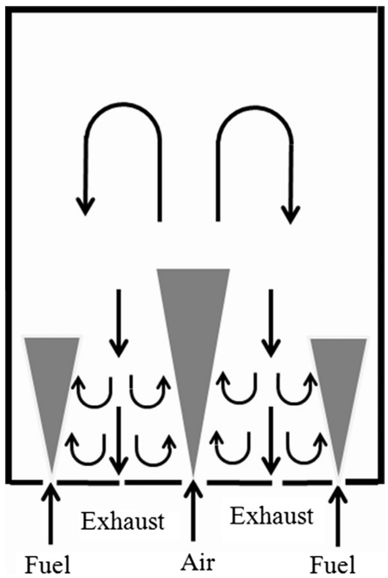

Fig. 1. Sketch of a parallel jet burner.

From the aspect of pollution, there are many studies on the mechanisms and characteristics of NO_x formation in the MILD combustion regime [6–8], but few systematic studies have investigated CO formation. The mechanisms of CO formation are closely related to the oxidation mechanisms of fuel in the MILD combustion regime. Numerical simulation is often used to study the mechanisms of combustion reactions. Mardani et al. studied the CO formation mechanisms under the MILD combustion conditions of a jet in hot coflow (JHC) through a zero-dimensional well-stirred reactor (WSR) analysis [9]. These researchers claimed that the ethane oxidation pathway (i.e., $CH_3 \rightarrow C_2H_6 \rightarrow C_2H_5 \rightarrow C_2H_4 \rightarrow C_2H_3 \rightarrow C_2H_2 \rightarrow CO$) had a significant effect on the CO formation under MILD conditions; thus, the rate of the traditional methane oxidation route (i.e., $CH_3 \rightarrow CH_2O \rightarrow HCO \rightarrow CO$) and ethane route are the keys to an increase in the CO concentration with increasing O_2 concentration. However, the reasons for the variation in the CO emission with the other parameters, such as the entrainment ratio (Kv), the equivalence ratio (ϕ), and the inlet temperature (T_{in}), were not provided in their reports. de Joannon et al. simulated MILD combustion under the conditions of hot-fuel-diluted-fuel [10] and hot-oxidant-diluted-fuel [11] using opposed diffusion flame (OPPDIF) and found that the reaction region is thickened and that the pyrolysis region is depressed in MILD combustion, which are necessary conditions to achieve distributed combustion and colorless combustion. In the post-combustion zone, dilution exerts a more significant effect on CO oxidation due to its stronger sensitivity to the concentration of the species, which implies that an increase in the entrainment ratio (Kv) is conducive to the conversion of CO to CO_2. The oxidative reforming process can depress pyrolytic recombination, which is the main channel of heavier carbonaceous products. This finding means that the paths of CO formation from heavier carbonaceous compounds are weakened in the MILD combustion regime. However, the mechanisms of CO formation were not provided in these studies because the researchers focused on the outstanding characteristics of MILD combustion compared with traditional diffusion flame. These researchers also indicated that the kinetic mechanisms GRI 3.0 are appropriate for the prediction of MILD combustion under diluted and pre-heated conditions.

The behavior of CO formation is observed in some MILD combustion studies. Shim et al. found that CO emissions increase with an increasing equivalence ratio in MILD combustion [12]. Cavigiolo et al. reported that the CO emissions decrease during the transition from traditional combustion to MILD combustion with an increase in the entrainment ratio after a temporary limited peak of CO emissions [13]. Derudi et al. observed a similar phenomenon using COG (coke oven gas) as the fuel in his experiments of MILD combustion [14]. Veríssimo claimed that CO emissions increase with an increase in the air inlet velocity [15]. The studies on CO emissions conducted by Yu He showed that CO emissions increase with an increase in the inlet momentum rates of the fuel and air streams [16]. Using perfectly stirred reactors (PSR) to simulate MILD combustion, Yu showed that the entrainment ratio has a minimal effect on CO formation in MILD combustion with a high dilution of reactants. He also revealed that the CO emission decreases when increasing the hydrogen content in the fuels [17]. Dally et al. showed that the concentration of CO decreases with a reduction in the O_2 concentration in the furnace. These researchers suggested that the mechanisms of CO formation in the MILD combustion regime are different from those in the traditional combustion regime but did not provide these new mechanisms [18]. Christo and Dally indicated that the CO distribution demonstrates an unusual behavior: the CO concentration increases rather than decreases at high O_2 concentrations and temperatures, which should be conducive to the conversion of CO to CO_2 in the traditional combustion regime [19]. The above results indicate that the entrainment ratio (Kv), the equivalence ratio (ϕ), and the inlet temperature (T_{in}) can impact CO formation in the MILD combustion regime, but these impacts have not been quantifiably discussed or systematically studied, and the kinetic mechanisms of these impacts remain unclear.

Recently, MILD combustion with ambient temperature air, which greatly extends the application area of MILD combustion technology because of the absence of heat exchangers, was achieved using a parallel jet burner [20], as shown in Fig. 1. This type of burner has been widely used to study various characteristics of MILD combustion, such as the operational characteristics [20], the effects of the fuel mixture [21], the effect of sawdust as the fuel [12], and the combination of MILD and oxy-fuel combustion [22]. As shown in Fig. 1, fuel, air, and exhaust gas ports were placed on the bottom of the furnace. The air stream feeds into the furnace through the central port, the fuel stream goes through the outermost ports, and the exhaust gas flows into the furnace through the middle ports. The aim of this arrangement is to make the fuel and air streams entrain the hot exhaust gas simultaneously before their mixing, which means that both the fuel and the oxidant are simultaneously preheated and diluted by the hot exhaust gas. Abtahizadeh et al. studied MILD combustion in this construct using a numerical model comprised of the combination of opposed

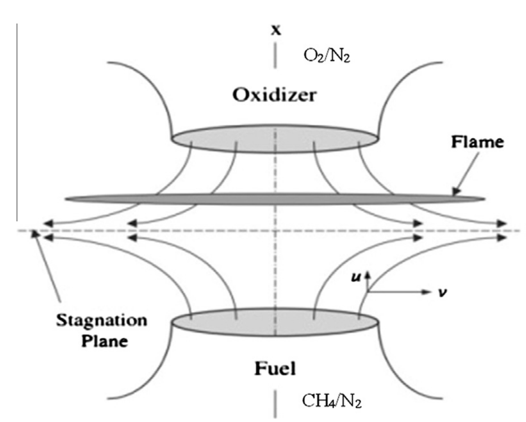

Fig. 2. Sketch of the opposed diffusion flame with simultaneously diluted and preheated oxidant and fuel.