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The effects of water addition on the laminar flame speeds of CO/H₂/O₂/H₂O mixtures

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ABSTRACT

The effects of H₂O addition and H₂ content on the laminar flame speeds of CO/H₂/O₂/H₂O mixtures were studied experimentally and theoretically. The laminar flame speeds were measured at various CO/H₂ ratios (100/0, 95/5, 85/15, 75/25, 50/50) and H₂O concentrations (0–60% in the mixtures) using an improved Bunsen burner method. The addition of water affected the laminar flame speeds of the mixtures by changing its thermal properties and altering the chemical kinetics of the combustion reaction. When the H₂ content was lower than 15%, the laminar flame speeds first increased and then decreased as the H₂O content increased. When the H₂ content was greater than 15%, the laminar flame speeds decreased with increasing H₂O content. The chemical effects (direct reaction effects and three-body effects) of H₂O addition on the laminar flame speeds were analyzed using CHEMKIN package. The direct reaction effects of H₂O addition present a promoting effect on CO/H₂ combustion (for H₂ content of 0–50%). However, adding large amounts of H₂O had a complex effect overall because of its impact on the three-body reaction which inhibited combustion. The three-body effect of H₂O addition decreased the concentration of free radicals (H, OH, and O) in the chemical reaction zone, caused the flame front to move downstream, and changed the HO₂ consumption pathway.

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Introduction

Oxy-fuel combustion technology offers the potential of cleaner combustion for power generation applications with relatively higher efficiency and lower cost of CO₂ capture in comparison with those of other carbon capture technologies [1–3]. Oxy-fuel combustion technology uses pure oxygen as the oxidant, compared to conventional fossil fuel combustion uses air—eliminating the dilution of N₂ (approximately 79% by

volume in air). H₂O or recycled flue gas (CO₂) is necessarily added to the combustion chamber to moderate the high flame temperature that would result from combustion in pure oxygen. The flue gas of hydrocarbon fuel combustion consists of only H₂O and CO₂, a high concentration of CO₂ can be obtained directly by cooling the flue gas. As well as being permanently stored in deep geological formations, compressed CO₂ can be used for enhanced oil recovery or as a raw material for chemical synthesis.

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Recently, many scholars have proposed water dilution oxy-fuel combustion, it is regarded as the next generation oxy-fuel combustion technology. Anderson et al. [4–6] proposed an efficient water cycle for power generation in which steam is directly injected into a pressurized pure oxygen flame to generate a high-temperature, high-pressure multi-working fluid ($\text{H}_2\text{O}/\text{CO}_2$ mixture). Salvador [7] and Seepana et al. [8] presented an atmospheric oxy-steam combustion technology that burns hydrocarbon fuel under $\text{O}_2/\text{H}_2\text{O}$ atmosphere in the boiler. Such $\text{O}_2/\text{H}_2\text{O}$ combustion technology has been reported to have many advantages over O_2/CO_2 combustion technology with flue gas recycle [9–11]. For example, using H_2O instead of flue gas recycle is simpler, requires less energy, and H_2O also chemically promotes of the combustion of CO. High water vapor concentration in the combustion is the distinct characteristics of $\text{O}_2/\text{H}_2\text{O}$ combustion. Water addition decreases the flame temperature, changes the chemical reaction process, and alters the concentration of free radicals in the flame.

CO and H_2 are the main components of gasification gas (syngas), which is regarded as a promising clean energy mainly derived from the gasification of coal or biomass [12–16]. The combustion characteristics and oxidation mechanism of CO/ H_2 are the fundamental basis for the efficient use of hydrocarbon fuel. The effects of different diluent gases (CO_2 , N_2 , and H_2O) and pressure on CO/ H_2 /air combustion have been studied experimentally and theoretically [17–30]. Specifically focusing on flame characteristics, as well as the elementary reactions. The effects of diluent gas can be attributed to the following aspects: dilution effect, thermodynamic and transport effect, chemical effect and radiation effect [31–34]. As noted above, the addition of H_2O with its high heat capacity is known to lower flame temperature and also flame speed. While a small amount of H_2O can greatly increase the combustion of pure CO (without H_2) [35,36]. This is because H_2O is involved in the reaction $\text{H}_2\text{O} + \text{O} = 2\text{OH}$ to produce OH radical which then promote the consumption of CO by the reaction $\text{CO} + \text{OH} = \text{CO}_2 + \text{H}$ [23,31,37,38]. Competition between the thermal and chemical effects of adding H_2O results in different change trend on the laminar flame speed of CO/ H_2 /air that depend on the CO/ H_2 ratio as the amount of H_2O added is increased. For CO-rich conditions, the laminar flame speeds of CO/ H_2 /air mixtures has been reported to first increase and then decrease as the concentration of H_2O is increased. Meanwhile, for CO-lean conditions, the laminar flame speed decreased linearly as the concentration of H_2O is increased [39,40]. The addition of H_2O improve the reaction rate of $\text{H}_2\text{O} + \text{O} = 2\text{OH}$ and decrease the concentration of O radicals in the flame, which in turn decrease the reaction rate of $\text{H}_2 + \text{O} = \text{H} + \text{OH}$. Therefore, the chemical effect of adding H_2O on CO/ H_2 combustion was inhibited at high concentration of H_2 [31,41].

The three-body collision coefficient of H_2O is 10 times larger than that of N_2 [42–44]. Thus, adding H_2O increases the reaction rate of three-body reaction. The reaction rate of $\text{H} + \text{O}_2 (+\text{M}) = \text{HO}_2 (+\text{M})$ was improved by H_2O addition for CO/ H_2 /Air flame. Here, H_2O addition hinders the diffusion of H radical produced in the flame zone into the upstream, and increases the relative content of HO_2 in the flame. In this way, the addition of H_2O changes the flame structure and the chemical reaction pathway of combustion [23,37].

The addition of H_2O changes the chemical reaction pathway and the concentration of free radicals of CO/ H_2 combustion. However, the effects of water vapor addition on the laminar flame speeds are difference for low and high H_2 content. The majority of existing CO/ H_2 flame propagation data has been derived in air atmosphere, and the water vapor content is low (no higher than 40% in the fuel mixture) except the study of Sun et al. [41]. As a result, there is limited amount of experimental data available of CO/ H_2 with high H_2O concentrations for chemical mechanism validation and optimization [45]. The effects of water addition on the flame characteristics of CO/ H_2 under $\text{O}_2/\text{H}_2\text{O}$ atmosphere remains unclear.

Therefore, this study measures the laminar flame speeds of CO/ H_2 / $\text{O}_2/\text{H}_2\text{O}$ mixtures with various concentrations of H_2O . The effects of H_2O addition on the concentration of free radicals in the flame zone under different CO/ H_2 ratios are also analyzed. A chemical kinetics simulation is also carried out to investigate the effects of H_2O addition on the elementary reactions of CO/ H_2 combustion. This investigation also includes an analysis of the direct reaction effects and the three-body effects of H_2O addition in CO/ H_2 / $\text{O}_2/\text{H}_2\text{O}$ flame.

Experimental and numerical methods

Experimental approach

An improved Bunsen burner setup, shown in Fig. 1 and described in full elsewhere [41], was employed to measure and calculate the laminar flame speeds of CO/ H_2 in $\text{O}_2/\text{H}_2\text{O}$ atmospheres. Smooth-contoured, high-contraction-ratio nozzles with outlet diameters of 3, 6, and 9 mm were used. The 3 mm diameter nozzle was only used for low water vapor content and high H_2 content conditions. A high contraction ratio ensured a uniform velocity distribution at the outlet and improved the stability of the flame. The boundary layer growth is suppressed compared to a straight tube and ensure

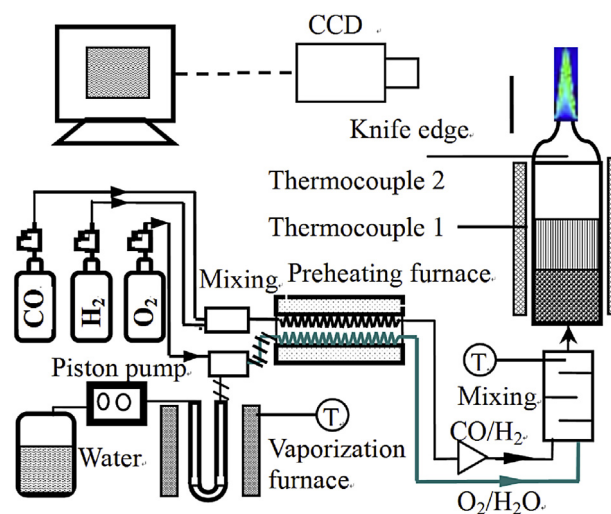


Fig. 1 – Schematic diagram of the Bunsen burner experimental system.

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