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The chemical mechanism of steam's effect on the temperature in methane oxy-steam combustion

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ABSTRACT

A numerical study with a detailed chemistry mechanism has been conducted to investigate the chemical effects of steam on the temperature in methane oxy-steam combustion; steam is used to moderate the high flame temperature produced by combustion of the fuel using oxygen. The temperature profiles of the oxy-steam combustion are consistent with those of traditional combustion when the mole fraction of steam in the oxidant is 72.5%. The comparisons between the maximum temperatures when steam is added and the corresponding artificial material X addition reveal that when the mole fraction of H_2O (or X) is between 0.60 and 0.66, the overall chemical effects of the steam peak. High steam concentration in the atmosphere enhances the three-body reaction, raises the concentration of OH, and lowers the concentration of H during oxy-steam combustion, in contrast to traditional combustion. Consequently, when the steam's mole fraction is between 0.5 and 0.7, the three-body reaction ($H + O_2 + H_2O \Longleftrightarrow HO_2 + H_2O$) (R35) is the key elementary reaction that determines the combustion temperature during oxy-steam combustion; this reaction also provides sufficient HO_2 to R287, giving R287 the highest heat release rate. When the steam mole fraction exceeds 0.75, the reduced oxygen mole fraction enhances the rate of CO production. Concurrently, R38 is the key elementary reaction for determining the combustion temperature because it supplies a large amount of radical OH species. Therefore, R99 dominates R287 and has the highest heat release rate. When the steam mole fraction is 0.725, R35 and R38 play a very important role affecting the combustion temperature; R99 makes the largest contribution to temperature, while R287 and R43 also make significant contributions to the temperature.

1. Introduction

Climate change is evident because the average temperatures of worldwide oceans and air have increased alongside the widespread melting of ice and snow and rising sea levels [1]. In 2007, IPCC [2] noted that the human activities contributing to global warming are mainly attributed to fossil fuel combustion. Therefore, seeking methods that can capture and store carbon dioxide has become an important challenge. CCS (Carbon Capture and Storage) is a promising technology that addresses global climate change [3]. For the carbon dioxide removal process, there are three main approaches for CCS: pre-combustion, post-combustion, and oxy-fuel.

Oxy-fuel is considered one of the promising methods for carbon dioxide emission abatement due to its low technological risk for industrialization [4]. A current example of oxy-fuel combustion is O_2/CO_2 recycled combustion. In this combustion mode, the fuel combustion occurs in mixtures of oxygen and recycled flue gas instead of air, ensuring that the CO_2 volume concentration exceeds 90% in the exhaust gas. According to Seepana [5], oxy-steam combustion is a combustion in which steam, instead of N_2 or CO_2, is used to moderate the high temperature produced by fuel combustion with oxygen. Oxy-steam combustion has numerous advantages over O_2/CO_2 recycled combustion, such as its compact system, ease of operation, small geometric size, and energy savings. Therefore, oxy-steam combustion technology may become a next-generation oxy-fuel combustion technology.

Oxy-steam combustion is different from conventional and O_2/CO_2 recycled combustion because the physicochemical properties of H_2O are very different from those of N_2 or CO_2 (Table 1). The steam can participate in the combustion reaction because its active chemical properties can change the reaction pathway and modulate the flame temperature. Richards et al. [6] studied the combustion performance of CO_2 and H_2O diluted oxy-fuel combustion using numerical calculations and experiments. The computational results indicated the required residence time in a CO_2 diluted

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Table 1
Comparison of physicochemical properties at 1000 K, 0.1 MPa.

Gas	Density (mol/m^3)	Cv (J/mol ∗ K)	Cp (J/mol ∗ K)	Therm. Cond. (W/m ∗ K)	ρc_p (J/ m^3 ∗ K)	Therm. Diff. (m^2/s)
H_2O	12.03	32.963	41.293	0.097085	496.754	0.000195
CO_2	12.025	46	54.322	0.070571	653.222	0.000108
N_2	12.023	24.386	32.703	0.065991	393.188	0.000168

system is 5 to 7 times greater, and the equilibrium CO levels are higher than those in H_2O diluted system; full-scale H_2O diluted oxy-fuel combustion experiments revealed that CO levels are higher than the equilibrium CO levels but are reasonable considering the low levels of excess oxygen. Moreover, there are few studies describing the combustion performance of oxy-steam combustion. However, there are numerous simulation studies [7–14] of the effect of diluents during conventional combustion. Park [15] studied a methane-air counter-flow diffusion flame with CO_2, H_2O, and N_2 additives. Although the heat capacity of steam (H_2O) is the highest among these three additives, the largest reduction in temperature occurs when CO_2 is added due to the super-balanced effect of H_2O; this effect offsets steam's heat absorption capacity. Park [16] researched mild combustion with steam additives using numerical simulations. According to the results, the maximum flame and oxidant temperatures are related. The combustion mode changes from high-temperature to mild when the fraction of steam exceeds 0.7. Jeong Park [17] studied the flame structure and pollutant emission from a CH_4/air diffusion flame with hydrogen and steam additives, reporting that the maximum flame temperature increases with increased hydrogen and decreased steam fractions; steam can regulate the flame structure by participating in the radical chain reaction. The maximum flame temperature when steam is added far exceeds that in the case of X addition when steam's mole fraction is 0.1. The chemical effect of steam promotes OH and restrains O and H radical formation via $O + H_2O \Longleftrightarrow OH + OH$. Boushaki [18] studied the propagation velocity of a CH_4/air flame with added H_2 and H_2O. Numerical simulations were conducted with COSILAB to study the 1D premix flame using the GRI 3.0 mechanism. Adding steam reduces the velocity of flame and the maximum flame temperature. The studies above focused mainly on the effects of steam as an additive, i.e., the effects of low steam concentrations on traditional combustion. However, the effects of high steam concentrations on oxy-steam combustion remain poorly understood.

When oxy-steam combustion is used to retrofit conventional boilers, matching the temperature profile between oxy-steam combustion and traditional combustion must be considered. Concurrently, the oxy-steam combustion temperature should also be controlled to remain in the appropriate range dictated by material limitations. Sivaji Seepana [5] reported that the different temperature profiles in furnaces for the oxy-steam combustion and traditional combustion match when the mass ratio of steam and oxygen is 36:64, but detailed calculations and experimental verifications were not provided. Moreover, few studies have been conducted regarding the flame temperature during oxy-steam combustion. Studying the chemical effect of steam addition on the flame temperature during oxy-steam combustion may help to spread the application of oxy-steam combustion technology.

In this work, the temperature profile comparison between CH_4-O_2/H_2O and CH_4-air was studied to identify the proper ratio of oxygen to steam to match the temperature profiles of the above two modes. Artificial material X has same physical properties as steam and is chemically inert; it was adopted to examine the overall impact of steam's chemical properties on the flame temperature. A sensitivity analysis was also used to study the chemical mechanism of steam's effect on the temperature during methane oxy-steam combustion.

2. Numerical simulation methods

In the current study, the opposed diffusion flame that is generally used to analyze the chemical kinetic mechanisms of the fuel combustion was employed to study both oxy-steam and conventional combustion processes. A geographical description of the opposed diffusion flame is displayed in Fig. 1. The distance between two nozzles is 0.75 cm. The initial temperatures of the fuel and oxidizer sides are 330 K and 900 K, respectively. The strain rate (α) is 408 s^{-1}. $\left(\alpha = \frac{2(-u_o)}{L}\left[1 + \frac{u_F}{(-u_o)}\sqrt{\frac{\rho_F}{\rho_o}}\right]\right)$. Thermal diffusion was accounted for and the mixture-averaged was chosen as the transport equation.

Due to the axisymmetry of the opposing jet configuration, the flow reaction equations are one-dimensional and can be written as (Kee [19], Lutz [20]) the mass continuity equation:

$$\frac{dU}{dx} + \frac{2\rho v}{r} = 0 \tag{1}$$

where U is axial mass flux, ρ is density, v is the radical velocity, x is the axial direction, and r is the radical direction.

The radial momentum equation is as follows:

$$U\frac{dv}{dx} - \frac{d}{dx}\left[\mu\frac{dv}{dx}\right] + \frac{3\rho v^2}{r} + \frac{\partial p}{\partial r} = 0 \tag{2}$$

where p is the pressure

The species conservation equation is the following:

$$U\frac{dY_k}{dx} + \frac{d}{dx}(\rho Y_k V_k) - \dot{w}_k W_k = 0, \quad k = 1, \ldots, K \tag{3}$$

The energy conservation equation is as follows:

$$Uc_p\frac{dT}{dx} - \frac{d}{dx}\left(\lambda\frac{dT}{dx}\right) + \rho\sum_k c_{pk}Y_k V_k\frac{dT}{dx} + \sum_k h_k\dot{w}k - \dot{q}_r = 0 \tag{4}$$

where Y_k is the mass fraction, V_k is the diffusion velocity, and $\dot{q}_r$ is the radiation term. Based on the optically thin approximation, the radiation term is calculated as:

$$q_r = -4\sigma k_p(T^4 - T_\infty^4) \tag{5}$$

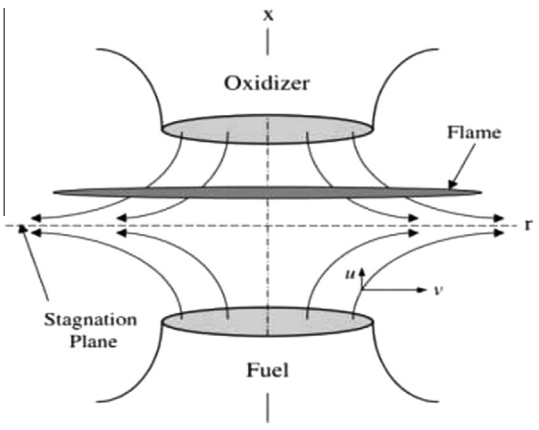

Fig. 1. A geographical description of the opposed diffusion flame.