Energy xxx (2015) 1–13

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy

Effects of flue gas recirculation on the premixed oxy-methane flames in atmospheric condition

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ARTICLE INFO

Article history:
Received 11 January 2015
Received in revised form
6 June 2015
Accepted 9 June 2015
Available online xxx

Keywords:
Oxy-fuel
Oxy-combustion
Fluegas
Flame structure
Laminar burning velocity

ABSTRACT

This numerical study investigates the flame characteristics of premixed methane with various dilutions in order to simulate oxy-combustion of hydrocarbon fuels with flue gas recirculation system. In general, a recirculated flue gas consists of high concentration CO_2/H_2O and high gas temperature. The effect of various diluent gases on laminar burning velocity and adiabatic flame temperature is discussed via using Chemkin-pro simulation. By observing the resultant flame temperature and species concentration profiles one can identify that the flame front shifts, and the concentration profiles of major chemical reaction radicals varies, indicating the change of flame structure and flame chemical reaction paths. The dominant initial consumption reaction step of methane shifts from R53 ($H + CH_4 = CH_3 + H_2$) to R98 ($OH + CH_4 = CH_3 + H_2O$) when nitrogen is replaced by the recirculated gases. H and OH radical concentration would be influenced in various diluent gas cases, so that it leads to affect hydrogen formation and methane consumption. It is because that the chemical effects of the recirculated gases change the chemical reaction of the oxy-fuel combustion, and further affect reaction rate, species and radical concentrations.

1. Introduction

To curb the increasing GHG (greenhouse gas) emission, such as carbon dioxide (CO_2) and methane (CH_4), pertinent and promising implementations are proposed to achieve the mission of GHG emission mitigation. Several strategies for the reduction and capture of carbon dioxide from industrial power plants are being considered. In general, the carbon dioxide concentration in conventional coal-air combustion flue gas is low, so that its in-situ storage is not economically and practically feasible. The concept of combined oxy-fuel combustion recycling with CCS (carbon capture and sequestration) has been the most attentive scheme [1]. The oxy-fuel combustion is the method of using pure oxygen or a mixture of oxygen and recycled flue gas as an oxidant to generate the product gas composed of carbon dioxide and water steam near stoichiometric condition [2]. Theoretically, it enables to produce highly concentrated carbon dioxide flue gas through the water condensing treatment, and it has the potentials in reutilization and sequestration of carbon dioxide. Nowadays, to retrofit the traditional fossil fuel fired power plant for oxy-combustion has been considered one of the cost-effective and feasible implements [3,4] to promote this technology in industries.

Nevertheless, the difference in thermal properties of nitrogen and carbon dioxide results in significantly different flame behaviors of the oxy-fuel combustion from conventional air combustion [5]. Several studies have reported that the recirculated carbon dioxide participates in the chemical reaction instead of acting as an inert gas in oxy-enriched combustion. Indeed, carbon dioxide and water steam as diluent gas in hydrocarbon combustion would alter flame behaviors via the following three mechanisms: (a) dilution effect caused by the reduction in reactants concentration in the reactive mixture; (b) thermal effect due to the absorption of partial heat release by the diluents, leading to a change in flame temperature; (c) chemical effect due to the activity of the diluents that may alter some reactions pathways.

Wang et al. [6] numerically examined the combustion feature of pulverized coal in a CO_2/O_2 atmosphere over a range of CO_2-to-O_2 mole ratios between 2.23 and 3.65 in early stage. Kimura et al. [7] discovered that the ignition delay and flame instability would

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http://dx.doi.org/10.1016/j.energy.2015.06.032
0360-5442/

occur in oxy-fuel combustion condition, and proposed that an increase of gas temperature and oxygen concentration in flue gas can mitigate the combustion instability. Besides, an increase of steam percentage in flue gas also can improve the oxy-fuel combustion efficiency. Ditaranto and Hals [8] stated that, in order to attain an adiabatic flame temperature similar to that in fuel-air combustion, oxygen volumetric concentration should be increased to at least 30% in their studies of CO_2/O_2 and methane premixed flame. Riaza et al. [9] mentioned that the ignition temperature was higher and the burnout velocity was lower in an atmospheric oxy-fuel condition ($21\%O_2 + 79\%CO_2$) than in air condition. This was due to the higher specific heat of CO_2 compared to N_2 and the lower diffusivity of O_2 in CO_2 than in N_2. Payne et al. [10] used a pilot-scale furnace to measure the gas emissions of oxy-combustion with dry and wet flue gas recirculation system. It is noted that the reduction of NO_x emission in dry flue gas recirculation system approached to 70% when the CO_2/O_2 mole fraction was 2.7. However, NO_x emission in wet flue gas recirculation decreased 83% when the $(CO_2 + H_2O)/O_2$ mole fraction was 3.2. In addition, the combustion efficiency of wet flue gas recirculation is higher than that of dry flue gas recirculation due to OH radical enhancement via H_2O pre-dissociation in a high temperature condition. Compared to nitrogen, the presence of carbon dioxide and water steam leads to an alteration of the chemical pathway. Haler et al. [11] experimentally and numerically investigated the flame behaviors of methane/air in different dilutions of CO_2, N_2, and CO_2–N_2 ($71.6\%N_2 + 28.4\%\ CO_2$). It was found that CO_2-dilution has inherently high thermal capacity compared to N_2-dilution, but also induces CO_2 dissociation.

Considered the effect of CO_2-dilution in chemical reaction of premixed hydrocarbon flames, Liu et al. [12] used fictitious carbon dioxide (CO_2(A)), which was artificially assumed to only possess identical thermal and transport properties as CO_2 but is excluded from chemical reactions, to compare with the real carbon dioxide results. It turned out that the flame burning velocity with fictitious CO_2(A) is lower than that with real CO_2. They attributed that CO_2 participates in the chemical reactions primarily through $CO_2 + H$═ $CO + OH$ (R99), and leads to reduction of laminar burning velocity. Corresponding to R99, significantly higher CO concentration was found in oxy-fuel combustion than in air combustion [13]. Park et al. [14] studied the effects of CO_2 dilution on methane-air flames and concluded that the addition of CO_2 influences the chemical flame structure. Similarly, Mazas et al. [15] investigated the effects of water steam addition on the laminar burning velocity of oxygen-enriched methane flames. It was found that water steam addition has a significant chemical effect on the burning velocity of methane-air flames, especially in lean and near-stoichiometric conditions.

Accordingly, the existence of recirculated carbon dioxide and water steam in oxy-fuel combustion certainly would induce chemical effect of premixed flame and modify flame characteristics and structure. Parameters, such as flue gas recirculation ratio, flue gas temperature as well as flue gas contents, are engaged to influence oxy-enriched and oxy-fuel combustion characteristics. These parameters are crucial in the design of oxy-enriched or oxy-fuel combustor. Although there is considerable literature on oxy-fuel combustion, systematic studies of physical and chemical flame structures of the oxy-fuel combustion under various flue gas recirculation conditions have not been reported and documented. This study would numerically examine the effects of flue gas additions on key flame characteristics, such as adiabatic flame temperature and flame burning velocity of methane/oxygen-flue gas combustion as compared with methane/air combustion, to distinct the role of the recirculated flue gas in oxy-fuel combustion. Various recirculation ratios of nitrogen, carbon dioxide, water steam, and flue gas ($33\%CO_2 + 67\%H_2O$) dilution in oxy-methane premixed combustion are numerically considered. The flame structures of methane/air premixed combustion in various flue gas dilutions are also investigated to serve as the baseline data for comparison.

2. Methodology

For studies of the chemical effects of oxy-fuel combustion, numerical simulation is a cost-effective and high-performance implement to observe the insight of flame structure and flame characteristics. Among currently available numerical mechanisms, GRI-Mech. 3.0 is extensively and intensively used in numerical analysis of oxy-methane combustion. For instance, Liu et al. [12] numerically investigated the chemical effects of carbon dioxide in oxy-fuel condition via GRI-Mech. 3.0. Mazas et al. [15] numerically investigated the effects of water steam addition on the laminar burning velocity of oxygen-enriched methane flames using GRI-Mech. 3.0, while Watanabe et al. [16] used GRI-Mech. 3.0 to examine the NOx formation and reduction mechanisms in staged oxy-fuel combustion and in air combustion. However, a modified GRI-Mech 3.0 is sometime applied in specific researches of oxy-fuel combustion. Watanabe et al. [17] used the modified GRI-Mech 3.0 [18] to discuss the impact of carbon dioxide on methane oxidation and hydrogen formation in fuel-rich oxy-combustion. The modified GRI-Mech. 3.0 involves 97 species and 779 elementary reactions that are larger than those in original GRI-Mech. 3.0. Abián et al. [19] used another modified mechanism, which consists of 128 species and 924 elementary reactions [20], to observe the impact of CO_2 and H_2O concentration on the oxidation process of CO. Nonetheless, the modified GRI-Mech 3.0 with larger species and reaction steps is usually designed and optimized for specific purpose and is generally more time-consuming and numerically unstable compared with GRI-Mech. 3.0. In this study, for general comparisons of the different oxy-methane and methane-air combustions with various flue gas dilution conditions, the unmodified GRI-Mech. 3.0 will be used with proper validations in the oxy-fuel combustion simulation.

2.1. Numerical methods

The PREMIX code of CHEMKIN Collection is used to calculate the adiabatic, unstrained, free propagation velocities of the CH_4 laminar premixed flames. It solves the equations governing steady, isobaric, quasi-one-dimensional flame propagation. For a freely propagating flame, the mass flow rate is an eigenvalue and must be determined as part of the solution. To obtain the accurate flame speed, the boundaries should be sufficiently far from the flame to avoid temperature and species gradients at the boundaries. In addition, the adiabatic flame temperature is calculated by using the EQUIL code of CHEMKIN Collection. An initial reactant mixture is specified and equilibrium of constant enthalpy and constant pressure is constrained.

As to the chemical kinetics, the GRI-Mech 3.0 mechanism [21] composing of 53 chemical species and 325 reaction steps and detailed transport properties are used. The reaction rate constant is represented by the modified Arrhenius expression,

$$k = \overline{A}T^b \exp\left(\frac{-E_a}{RT}\right) \tag{1}$$

where $\overline{A}$ is the pre-exponential factor, b is the temperature exponent, and E_a is the activation energy. The chemical kinetics with CHEMKIN format is used in the code. Details of the chemical reaction rate formulation and CHEMKIN format can be found in the user's manual [22].

Please cite this article in press as: Li Y-H, et al., Effects of flue gas recirculation on the premixed oxy-methane flames in atmospheric condition, Energy (2015), http://dx.doi.org/10.1016/j.energy.2015.06.032