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Numerical study on the effects of oxygen enrichment on methane/air flames

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HIGHLIGHTS

- Effects of oxygen on flame thermal properties and NO production were studied.
- A bit of oxygen increased NO formation, but more oxygen decreased NO emission.
- Oxygen shows it significant effects in the pathways of CH_3 oxidation.

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ABSTRACT

In the study, we numerically simulated premixed laminar methane/air flames enriched by oxygen at flame equivalence ratios of 0.7, 1.0 and 1.2, and over a wide range of enrichment ratios from 0 to 0.79. The effects of oxygen enrichment on flame characteristics were studied through comparing global thermal properties, NO production and flame kinetics. With the addition of oxygen, the flame temperature gradient, inner layer temperature, and average heat release rate are consistently increased, and the flame thickness decreases. According to the predictions of NO emission, a small amount of oxygen addition increased NO production, whereas a large quantity of oxygen decreased NO emission. Moreover, we explored the kinetic effect of oxygen enrichment on flame reaction routes via flame kinetic analyses. The effect of oxygen enrichment was inconspicuous in the pyrolysis routes from CH_4 to CH_3, in which the related reactions were promoted coequally. Significant differences were found in the pathways of CH_3 oxidation, in which the reactions related to the consumption of O, OH, and H had been promoted significantly. Based on the analyses of the variations of reaction progress rate, we found the primary affecting routes of oxygen on methane/air flame. R38 and R84 played central roles in methane oxidation and they were promoted by oxygen addition and consequently contributed to the acceleration of the global reaction of enriched flames.

1. Introduction

Combustion processes are always taken placed at atmospheric condition, in which the atmospheric air consists of approximately 21% oxygen and 79% nitrogen by volume and only oxygen was used as the real oxidant. In order to achieve optimized combustion with the much higher efficiency, Oxygen-Enriched Combustion (OEC), which utilizes a high concentration of oxygen as the combustion oxidant compared to air, had obtained wide attention. Wu and his co-workers [1] studied the effects of oxygen concentration on the temperature, emissions, and fuel consumption of nature gas in a heating burner and found that the fuel efficiency and radiation heat transfer were increased with the increase in the oxygen concentration in the mixture and that the fuel consumption at the oxygen concentration of 30% was 26.1% less than that in the air with 21% oxygen by volume. Qiu and Hayden [2] made an experimental study in a gas-fired radiant burner and indicated that an increase of oxygen concentration offered 22–28% potential savings of natural gas consumption. Prieler et al. [3] studied the natural gas combustion under different oxygen concentrations and found that the maximum combustion efficiency of 67% was obtained for

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natural-gas combustion in pure oxygen, compared to 44%, which was obtained under oxygen volumetric concentration of 25%.

It was reported that the addition of oxygen could enhance the stability of flame. Li et al. [4] investigated the stretch extinction limits of CH_4/CO_2 mixture versus high-temperature O_2/CO_2 counterflow flames and found that the effect of oxygen concentration on the extinction limits of oxygen-enriched flame was significant. Merlo et al. [5] studied the combustion characteristics of turbulent swirling methane flames enriched by oxygen and found that the stability of flame and NO_x emissions increased significantly with oxygen addition.

Laminar flame velocity is one of the important global parameters of flame reactions. The laminar flame velocities of oxygen-enriched flames were experimentally and numerically studied extensively [6–8]. Cardona and Amell [6] found that the laminar flame velocity of biogas flames increased with the increase of oxygen concentration in oxygen-enriched air. de Persis and his coworkers [9] numerically and experimentally studied the laminar flame velocities of $CH_4/N_2/CO_2/O_2$ mixtures with the shadowgraph technique and indicated that the laminar flame velocity increased with the increase in the ratio of $O_2/(O_2 + N_2)$.

Compared to laminar flame velocity, heat release rate is another key property of flame. A fine distinction in heat release might lead to significant changes in the flame structure. Lafay et al. [10] studied the effects of hydrogen on the flame thickness of the mixture of methane and air by means of heat release analyses. Hu et al. [11] and Li et al [12] computed the heat contribution of flame reaction to the global heat released by the flame, and found the dominant reactions.

In previous studies, enrichment effects of oxygen on methane/air flames were generally focused on the macroscopic features, such as the engine performance and the flame velocity, but the thermal features of the flames were hardly found. We implemented a numerical prediction on the thermal properties of methane/air flames. The thermal structures of flame were computed in terms of the flame temperature gradient, inner layer flame temperature, flame thickness, heat release rate, and NO production was predicted as well. And then comparisons for the thermal properties of flame were made for methane/air flames with and without oxygen enrichment to find the effect of oxygen. To the best of our knowledge, reaction kinetic analyses of enriched flames were generally conducted to explore the variations in active species profiles, which were focused on the formations and consumptions of the radicals. We analyzed the kinetic role of oxygen enrichment by exploring flame reaction routes. The presence of oxygen enrichment is shown to enhance the generations of O, OH and H. The keys reactions were found through the analyses on reaction pathways and the variations of the progress rates of reactions. This work aims to provide some important data on the global thermal properties of enriched flames and present useful analyses in finding some clarifications for oxygen-enriched combustion promotion.

2. Flame modeling methods

Flame modeling of oxygen-enriched methane/air flame was performed by means of solving the governing conservation equations for one-dimensional freely propagating premixed flame with the PREMIX code of CHEMKIN II [13]. One-dimensional freely propagating premixed laminar flame was idealized and fully developed without heat loss. Flame propagation was generally governed by the properties of fuel-oxidizer mixtures, which was often used in modeling the flame characteristic under specified conditions.

The simulation started under the atmospheric conditions of the pressure P of 0.1 MPa and the initial temperature T_0 of 300 K and oxygen enrichment ratio ranged from 0 to 0.79. Oxygen enrichment ratio, α, is defined as the additional volumetric fraction of oxygen in air:

$$\alpha = \frac{n_{O_2}}{n_{air}} - 0.21, \tag{1}$$

where n_{O_2} and n_{air} respectively denote the volumetric fractions of O_2 and air. $n_{air} = n_{O_2} + n_{N_2}$, n_{N_2} is the volumetric fraction of nitrogen; 0.21 is the volumetric fraction of oxygen in normal air. Obviously, for the flame with $\alpha = 0.79$, combustion occurs in pure oxygen environment.

Flame equivalence ratio, ϕ, is defined as

$$\phi = \frac{n_{CH_4}/n_{air}}{FAR_{stoic}}, \tag{2}$$

where n_{CH_4} is the volumetric fractions of methane in the initial unburned mixture; FAR_{stoic} is the volumetric ratio of fuel to air under the stoichiometric condition and given as

$$FAR_{stoic} = \frac{\alpha + 0.21}{2}. \tag{3}$$

The hybrid time-integration and Newton-iteration were adopted in PREMIX code to solve the steady-state mass, species and energy conservation equations of premixed laminar flame and an adaptive mesh technique was adopted in the flame computation to ensure a fast convergence [12]. The initial computational grid point was defined as 10 and the allowable maximum grid amount was 500. The gradient and curvature were both set to be 0.1 to control the adaptive accuracy.

The adopted kinetic reaction mechanism was GRI 3.0 [14], which was a detailed kinetic reaction mechanism and widely used in modeling light hydrocarbon oxidation in air. GRI 3.0 consists of 325 elementary chemical reactions and 53 reactive species. Its accuracy had been proved in methane/air flames modeling [10,15–20].

Fig. 1 shows a validation of GRI 3.0 in predicting laminar flame velocities for methane/air flames with different oxygen enrichment ratios. The measurements of de Persis et al. [9] were plotted for comparison. The predictions obtained with GRI 3.0 were in good agreement with the measured results and the kinetic scheme of Shi et al. [21] was well consistent with laminar flame velocity predictions over the whole range of oxygen enrichment ratio. However, slight overestimations for San Diego mechanism [22] were found via above comparisons.

With the data of flame kinetic scheme, reactive specie transport properties, and GRI3.0 mechanism, the flame structures in terms of the distribution of flame temperature and reactive species could be

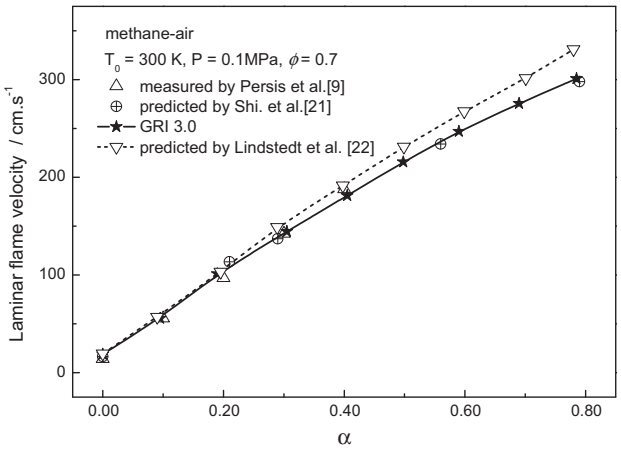

Fig. 1. Laminar flame velocity of methane/air versus oxygen enrichment ratio.