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Effects of equivalence ratio, H_2 and CO_2 addition on the heat release characteristics of premixed laminar biogas-hydrogen flame

Z.L. Wei [a,**], C.W. Leung [a,*], C.S. Cheung [a], Z.H. Huang [b]

[a] Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, China

[b] State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an 710049, China

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ABSTRACT

The effects of *equivalence ratio*, H_2 and CO_2 on the heat release characteristics of the premixed laminar biogas-hydrogen flame were investigated with the chemical kinetics simulation using the detailed chemical mechanism. The heat release rates, reaction rates and mole fractions of species of the BG50, BG75 and methane flames were calculated at different hydrogen additions (10%–50%) and equivalence ratios (0.8, 1.0, 1.2). The contributions of major elementary reactions were *obtained* based on the simulation data. The results show that $H + O_2 = OH + H$ is the major *endothermic* reaction for biogas-hydrogen flame, while $H + CH_3(+M) = CH_4(+M)$, $O + CH_3 = H + CH_2O$, $OH + H_2 = H + H_2O$, $O + CH_3 => H + H_2 + CO$ and $OH + CO = H + CO_2$ can always play significant roles in heat release. *$O + CH_3 = H + CH_2O$ and $O + CH_3 => H + H_2 + CO$* can consistently account for a relatively stable proportion of *total heat release*, meaning that the $O \times CH_3$ product can be an indicator to predict the total heat release. Due to the variation of O_2 concentration, the changes of major exothermic reactions are predominated by the equivalence ratio. Though the global heat release rate is maximum at stoichiometric condition, there exists more heat release in the high temperature zone at rich condition due to the exothermic recombination of radicals. The total heat release can be increased evidently with the H_2 addition which can induce the early heat release and enhance the peak heat release rate, and *the significances of $OH + H_2 = H + H_2O$ and $H + OH + M = H_2O + M$ on the total heat release are enhanced most evidently*. CO_2 exerts influences on heat release characteristics through its dilution/thermal effect and chemical effect. As CO_2 is introduced, the decreasing trend of the global heat release rate is dominated by the dilution/thermal effect, *and $H + CH_3(+M) = CH_4(+M)$, $OH + H_2 = H + H_2O$ and $2CH_3(+M) = C_2H_6(+M)$ become increasingly important* on the heat release.

* Corresponding author. Tel.: +86 852 2766 6651; fax: +852 23654703.
** Corresponding author.
E-mail addresses: zhilongwei.xjtu@gmail.com (Z.L. Wei), mmcwl@polyu.edu.hk (C.W. Leung).

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Introduction

With the increasing concerns over the global energy demand and the discharge of greenhouse gases (GHGs), the renewable and sustainable energy has been extensively studied in recent decades. Biogas, as a promising sustainable energy, can be produced by the wastes coming from agriculture, domestic sewage and landfills, and its short carbon cycle would not contribute to the increase of GHGs [1]. Thanks to its environmentally friendly features, biogas has been widely adopted as the fuel for heating facilities and vehicles in many countries. In Germany, biogas is mainly used for combined heat and power (CHP) generation, and the generated electrical power supplied to the national grid is increasing over the last few decades [2]. Meanwhile, European Union expects that the 10% of fuels used in the transportation system would be replaced with the biofuels by 2020 [3].

The main compositions of biogas are methane (CH_4) and carbon dioxide (CO_2), while water (H_2O), nitrogen (N_2) and hydrogen (H_2) can also account for a small proportion. Thanks to the different raw materials, the percentage of CH_4 in the biogas can reach up to 80%, while that of CO_2 varies between 20% and 60% [4–6]. It is obvious that the heating value of biogas is relatively lower than that of the natural gas due to the existence of CO_2. The lower heating value, as well as the thermal and chemical properties of CO_2, can restrict the utilization of biogas in the practical combustion facilities. For the sake of exploring the fuel characteristics of the biogas, related experiments and/or numerical simulation have been performed by several researchers. Dai et al. [7] conducted the experiments to investigate the flame stability of premixed biogas flames (CH_4 55%–70%) using the Reference Test Burner. Results show that high CO_2 concentration can bring about the unstable condition of "float off". Díaz-González et al. [8] experimentally determined the flame speeds of the biogas composed of 60% CH_4 and 40% CO_2, and discussed the effects of CO_2 on the flame structure and the radiation pattern. Anggono et al. [1,9] measured the laminar burning velocity of the biogas (66.4% CH_4 and 30.6% CO_2) using a fan-stirred combustion vessel, and found that CO_2 composition can lead to the narrower flammability and the decreased flame speed of the biogas-air mixture. In addition, some other researches were also performed experimentally or numerically to investigate the effects of CO_2 on the flame stability, flame speed and pollutant emissions using various methods [10–13]. Though the CO_2 in the biogas can reduce the pollutant emissions, its negative influences on the fuel characteristics were extensively confirmed by these studies.

In order to better utilize the biogas, the relatively poor fuel characteristics of biogas can be improved through blending it with other high quality fuel, such as liquid petroleum gas (LPG) and liquefied natural gas (LNG). Several researches have been carried out so as to explore the applicability of this method. Lee et al. [14] conducted the experiment to investigate the flame stabilities of biogas, biogas-CH_4 and biogas-C_3H_8 mixtures using the domestic appliances and swirl combustors. The improvement on the burning velocity and flame stability of biogas-mixed fuels are reported in their study. Cardona et al. [15] experimentally and numerically determined the laminar burning velocities of biogas (66% CH_4 and 34% CO_2) and the biogas-mixed fuel (50% biogas, 40% C_3H_8 and 10% H_2) at different equivalence ratios. Results show that the laminar flame speeds of biogas-mixed fuel are increased and this biogas-mixed fuel is eligible to be a substitute for natural gas. Lee et al. [16] performed another experiment to explore the interchangeabilities of biogas-LPG mixed fuels with respect to the application in domestic appliances, and found that the biogas-LPG can be applied directly to the existing facilities by varying the proportion of LPG suitably. These researches indicate that the blending fuel is a feasible method to improve the fuel characteristics of biogas. Hydrogen is an environmentally alternative energy and has been considered as an excellent addition to improve the fuel characteristics. Therefore, hydrogen addition can be a promising way to better utilize the biogas fuel. Leung et al. [17] experimentally studied the effects of hydrogen addition on the stability limits of the biogas diffusion flames. Results suggest that a small amount of hydrogen addition can significantly expand the stability range of the biogas diffusion flame. Zhang et al. [18] use the spark ignited engine to study the effects of hydrogen addition on the combustion instability of biogas fuel. It was concluded that the hydrogen addition can accelerate the heat release rate and improve the combustion stability of the biogas fuel. Zhen et al. [19,20] experimentally measured the heat flux of the biogas-hydrogen impingement flame and investigated the effects on the heat transfer characteristics of the biogas flames. The promotion of hydrogen enrichment on the flame stability and heat transfer performance are elucidated in these works. Though the fuel characteristics of biogas-hydrogen fuel have been investigated by several researches, much more fundamental studies should be carried out so as to establish the clear and comprehensive understandings of such a new blending fuel. Furthermore, heat release characteristics, as an important part of the fuel characteristics, are concerned with many significant fundamental parameters, such as heat release rate (HRR), chemical reaction rate and flame thickness, which not only play quite critical roles in several advanced combustion modes, such as HCCI and RCCI [21–23], but also affect the combustion process in the traditional combustion devices [24–26]. However, the heat release characteristics of the biogas with hydrogen addition have not been well understood, though several experiments have been performed with the power engines using the biogas-hydrogen as the fuel [27–29]. The information of the heat release characteristics can improve the comprehensive understandings of the biogas-hydrogen fuel, which makes for its applications in the practical combustion equipment. Meanwhile, the analysis on the heat release characteristics can facilitate to understand the mechanism of heat release and then help to find the method to control the heat release rate in the real combustion process. Hence the effects of equivalence ratios, H_2 and CO_2 on the heat release characteristics of the biogas-hydrogen fuel will be investigated in this study for the sake of providing some information to improve the understandings of such a new fuel.

Numerical simulations of premixed laminar biogas flames with hydrogen enrichment will be conducted to investigate the heat release characteristics in this study. The heat release rates, reaction rates and mole fractions of species of the biogas and methane flames will be calculated at different hydrogen additions and equivalence ratios. Additionally, the contributions of major elementary reactions will be calculated