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Ultra-lean combustion characteristics of premixed methane flames in a micro flow reactor with a controlled temperature profile

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Abstract

Experiments and computations for $CH_4/O_2/Xe$ and $CH_4/O_2/N_2$ mixtures at ultra-lean conditions using a novel vertical micro flow reactor with a controlled temperature profile were conducted. The performance of several chemical mechanisms was evaluated at equivalence ratios 0.3, 0.5, and 0.7, and at different dilution ratios by observing the weak flames. Comparisons between $CH_4/O_2/Xe$ and $CH_4/O_2/N_2$ flame locations indicated that $CH_4/O_2/Xe$ mixtures have a higher reactivity than $CH_4/O_2/N_2$ flames both experimentally and computationally. Furthermore, both experimental and computational results indicated that lower dilution and lower equivalence ratios increase reactivity. Comparisons between experimental and computational weak flame positions showed that computational results obtained with San Diego mechanism showed the best agreement to the experimental results compared to GRI-Mech 3.0 and AramcoMech 1.3. Comparison between $CH_4/O_2/Xe$ and $CH_4/O_2/N_2$ flame structures indicated that observable differences are seen between 1000 and 1100 K. Sensitivity analysis showed that OH radicals are important in determining the weak flame location. Reaction path and rate of production analysis showed that OH radicals are largely produced by (R1) $H + O_2 \Leftrightarrow OH + H$, and are inhibited by the third-body related reactions represented by (R10) $H + O_2 + M \Leftrightarrow HO_2 + M$. Since the third-body collision efficiency is larger for N_2 than Xe, it was shown that the reactivity becomes lower for N_2 mixtures than for Xe due to the larger effect of third-body reactions, which explained the difference in reactivity for Xe diluted and N_2 diluted flames.

Keywords: Micro flow reactor; Lean combustion; Xenon diluted flame; Flammability limit; Chemistry validation

1. Introduction

Although the flammability limit [1–3] and near-limit phenomena [4–6] of premixed flames have been extensively studied in the past, complete clarification has not been achieved yet, particu-

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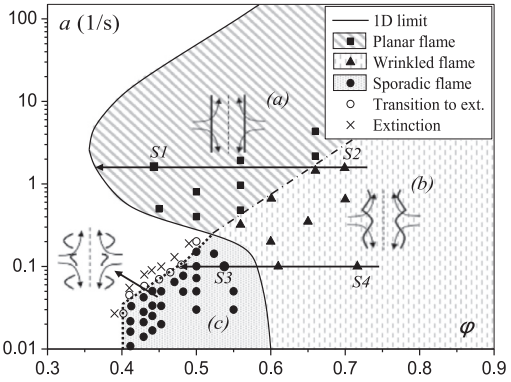

Fig. 1. Computational counterflow flame regime obtained by 3-D transient computations using a diffusive-thermal model [8].

larly for low-Lewis number premixed flames. Only recently have Takase et al. [7] succeeded in experimentally and computationally obtaining a transition from planar flames to ball-like flames at extremely low stretch rates by using $CH_4/O_2/Xe$ counterflow flames under microgravity. Subsequently, another study using 3-D transient computations by Fursenko et al. [8] on low-Lewis number premixed counterflow flames have also indicated the existence of an extended flammable region at lower stretch rates and at lower equivalence ratios than the extinction boundary of planar counterflow flames (see Fig. 1). In their studies, the extension of the flammable region was shown to be due to the formation of multiple ball-like flames, named sporadic flames [8]. In fact, microgravity experiments under atmospheric pressures for low-Lewis number premixed counterflow flames at extremely low stretch rates are scheduled for 2018 on the KIBO module of the International Space Station. Future investigations will be conducted in the region of sporadic flames at extremely low stretch with a long chemical time scale near the radiative extinction. At these conditions, the flame temperature becomes very low which is around 1000–1300 K due to radiative heat loss. Also, the mixtures investigated will be at even leaner conditions than the normal flammability limit. To conduct investigations on such conditions using computations, a fully validated chemistry at ultra-lean mixtures, and low temperatures under atmospheric pressure is necessary.

In general, detailed chemical mechanisms are validated in various flame configurations [9–14]. However, due to the experimental principles of each methodology, flame stabilization and the evaluations of a chemical mechanism at ultra-lean conditions are very difficult tasks. By using the microgravity environment, a study on the extinction boundary of near-limit counterflow flames have shown that the discrepancy between experimental and computational extinction points of counterflow flames become larger as the equivalence ratio ϕ is decreased down to very lean conditions [5], which indicated a further need for a valid chemical mechanism at ultra-lean and low temperature regions. Since microgravity environments are not easily accessible, we have employed the micro flow reactor with a controlled temperature profile in this study [15–18]. The micro flow reactor can be applied to near-limit or even outside of the flammability limit conditions due to the compensation of the heat loss by an external heater [19].

Past studies using the micro flow reactor with a controlled temperature profile have shown that at flame temperatures around the temperature region of radiative counterflow flame extinction, flames with weak luminescence called weak flames can be observed inside the micro flow reactor [15]. In this condition, the chemical time scale in the micro flow reactor is also on the same order as that of counterflow flames. Therefore, weak flames were chosen to be the focus of the present study.

Weak flames observed in the micro flow reactor have been studied from C0 up to C16 [16] fuels. A study on weak flames for gasoline primary reference fuel and toluene mixtures [17] by Hori et al. showed that the multi-stage oxidization is observed in the micro flow reactor, and investigation on the reactivity of the mixture could be conducted by comparing the weak flame locations. Furthermore, a quantitative agreement for the weak flame locations between the computational and experimental results were obtained, which demonstrated the capability of the micro flow reactor to validate chemical mechanisms. The quantitative effect of radical quenching at the quartz wall was also found to be negligible in the micro flow reactor [20,21]. Another study by Kamada et al. on the weak flames for natural gas components have shown that quantitative agreements between experimental and computational weak flame locations could be found for C2–C4 carbon number fuels [18]. However, a large discrepancy in the experimental and computational weak flame locations existed for CH_4/air flames at stoichiometric conditions [18].

The present study expands upon this study of CH_4 weak flames towards ultra-lean mixtures, and compares the experimental weak flame locations to computational weak flame locations obtained from multiple detailed chemical mechanisms. Moreover, the effect of the different diluents and third-body reactions on the weak flame locations will be discussed.

2. Experimental and computational methods

A schematic of the present experimental setup is shown in Fig. 2. A quartz tube with an inner diameter of 2 mm was placed vertically and used as a reactor channel. The tube was heated along the tube

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