H-TALIF measurement for wall radical quenching modelling in microscale combustion

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Abstract. Two-dimensional hydrogen atom (H) distribution in a CH₄/air premixed flame in a narrow channel was measured using a newly-developed two-photon absorption LIF (TALIF) setup with high efficiency 205 nm laser. The wall chemical effect of SUS321 and quartz surfaces on the H distribution in a methane flame was examined. Based on the measured H atom concentration near the wall, a radical quenching model focused on the H adsorption is proposed and the initial sticking coefficient (S₀) of H on SUS321 and quartz surfaces are estimated as 0.1 and 0.01, respectively. Sensitivity analysis of CO, HRR and species distributions with varying S₀ of H, O, OH, CH₃ were performed. It is found that the H adsorption should be dominant in the wall chemical effect on the methane flame.

1. Introduction

Flame-wall interaction (FWI) plays an important role in the near-wall flame behavior of internal combustion engines and gas turbines. The ignition process and emission can be greatly changed due to the FWI. Dreizler and Bohm [1] reviewed advanced laser diagnostic techniques to assess near-wall thermal, fluidic and chemical properties for the investigation of FWI. In the case of micro combustors for the portable power generation, FWI becomes more significant due to the large surface to volume ratio, resulting in flammability and flame stability problems. Flame quenching due to the thermal FWI in micro channels has been intensively studied to understand wall heat loss effects [2-6]. It was found that the flammability region shrinks as the wall heat loss increases with the downscaling, and the quenching distance, defined as the minimum channel height to hold a flame, decreases when the wall heat loss is reduced by external heating [4]. Also, unwanted flame instability phenomena such as the oscillating flame (also called FREI) and the spinning flame were observed in various micro combustors having different geometries [2-6].

Unlike the intensively-studied wall thermal effect, it was only recently that strong wall chemical effect in microscale combustion was observed [7-8] and examined quantitatively [9-10]. Miesse et al. [7] found that the quenching distance strongly depends on the wall material at high wall temperature (1000 °C). Saiki et al. [9-10] conducted OH planar laser induced fluorescence (OH-PLIF) measurements of a methane/air premixed flame in a quartz micro channel with/without alumina or metal coatings. They found that the near-wall OH concentration is significantly affected by the surface materials at high wall temperatures (≥800 °C). Raimondeau et al. [11] numerically examined the effect of wall radical quenching by arbitrarily setting all the initial sticking coefficients (S₀) for the adsorption of H, O, OH, CH₃ to 0~1.0. Saiki et al. [9-10] obtained S₀ over alumina (S₀=0), quartz (S₀=0.01) and metal (S₀=0.1) surfaces based on their OH-PLIF measurements.
Up to now, $S_0$ for the adsorption of different radicals is assumed to be the same for different radicals. This is because of limited quantitative information on the near-wall radical distribution other than OH. In the present study, the adsorption of H in the wall radical quenching was examined through the measurement of H atom concentration using newly-developed two-photon absorption LIF (H-TALIF) and numerical simulations assuming different $S_0$ for H, O, OH, CH$_3$.

2. Experimental Setup & Numerical Methods

Figure 1a shows the experimental setup for the examination of wall radical quenching using H-TALIF. A lifted CH$_4$/air premixed flame from the honeycomb burner is held in 3 mm-wide gap between two quartz plates. The bulk mean velocity and equivalence ratio $\phi$ for the mixture are 0.22 m/s (at 20 °C) and 0.95, respectively. A black quartz layer is fused to the back side of each quartz plate for the adsorption of thermal radiation from the IR heater. The wall temperature, $T_w$, is monitored by thin sheathed type-R thermocouple ($\phi$ 0.5 mm) in the plate. The wall surface is alternatively coated with ~100 nm-thick SUS321 film to change the chemical boundary while keeping the thermal boundary identical.

Observing H atom using the single-photon absorption LIF is difficult due to the strong absorption of VUV photons at 102 nm in other species in the air. Instead, the H atom in the flame is excited by two photons of 205.144 nm laser in TALIF, and the fluorescence at 656 nm is captured by the ICCD camera with a bandpass filter. Figure 1b shows newly-developed 615 nm→205 nm third harmonic generation (THG) setup for H-TALIF measurements. Unlike previous setups having poor THG efficiency (~2%) due to separate 615 nm and 307.5 nm optical paths [12-13], all THG optics in the present setup are arranged in a single axis through the implementation of a dual-wavelength wave plate and a walk-off compensation BBO crystal. As a result, alignment is much easier, and a THG efficiency as high as 9 % has been obtained, which makes the 2-D H-TALIF measurement possible. A laser sheet of 0.2 mm×3.0 mm is formed. The energy distribution in the laser sheet is calibrated beforehand by taking the TALIF signal of Kr gas with uniform concentration as the reference.

Two-dimensional numerical simulations were carried out in ANSYS Fluent 18.0 with employing GRI-Mech 3.0 as the gas phase reaction mechanism and the wall radical quenching model as the surface reaction mechanism. Beside the wall radical quenching model assuming equal $S_0$ for all H, O, OH, CH$_3$ adsorptions, the model assuming the adsorption of H only is also applied. The computation domain is half of the 3-mm-wide channel due to the symmetry and the boundaries are set to the same as in the present experiment. Details are described in our previous work [10]. Sensitivity analysis of the exhaust CO, heat release rate (HRR) and species distributions to the independently varying $S_0$ for H, O, OH, CH$_3$ was also performed, where the channel width is set to a smaller value of 0.7 mm to obtain stronger chemical effect.

Figure 1. (a) Experimental setup of H-TALIF measurement of CH$_4$/air premixed flame in a 3 mm-wide channel. (b) Schematic of 205 nm laser generation.
3. Results and Discussion

Figure 2 shows contours of normalized H molar concentration ($c_H/c_{H,max}$) measured through the H-TALIF being calibrated by the Kr-TALIF. Measured wall normal distributions of $c_H/c_{H,max}$ at $T_w = 1000 \degree C$ are plotted in Fig. 3 and compared with simulated distributions assuming either all H, O, OH, CH$_3$ adsorptions or H adsorption only. It is shown that $c_H/c_{H,max}$ over SUS321 is lower than that over quartz, so that SUS321 surface is more active than quartz in the adsorption of H. Simulated near-wall $c_H/c_{H,max}$ is very sensitive to $S_0$ and decreases gradually from $S_0 = 0$ (inert) to 0.1 (active). $c_H/c_{H,max}$ with assuming all radical adsorptions and only the H adsorption shows no big difference, which implies that H adsorption should be dominant in the wall chemical effect. By matching measured and simulated $c_H/c_{H,max}$, $S_0$ for SUS321 and quartz are estimated as 0.1 and 0.01, which agrees well with our previously obtained $S_0$ values based on the OH-PLIF measurement and the radical quenching model assuming equal $S_0$ of H, O, OH, CH$_3$ [9-10].

The importance of H adsorption is obvious through the above comparison, yet it is of concern that how sensitive the combustion field is to the adsorption of H and other radicals. Figure 4 shows the sensitivity results through simulations with varying $S_0$ of H, O, OH, CH$_3$ separately. It is found that both CO and heat release rate (HRR) are extremely sensitive to the adsorption of H, but not O, OH, CH$_3$. 35 % reduction in CO and 15 % improvement in HRR are obtained with decreasing $S_0$ of H from 0.1 to 0.001. Figure 5 compares CO and HRR in cases of all radical adsorption and single radical adsorption of H, O, OH, CH$_3$ each. Even if only the H adsorption is assumed, CO and HRR are deteriorated to the same level as all radical adsorptions.

As shown in Figs. 6ab of $c_H$ contours with/without the H adsorption, $c_H$ near the wall decreases drastically. It is shown in Fig. 6c of wall normal distributions that not only $c_H$ but also $c_{OH}$ and $c_O$
decreases with assuming only the H adsorption. This explains why our previously-obtained \( S_0 \) based on the OH-PLIF measurement and the equal \( S_0 \) model [9-10] could have the same value as here. The adsorption of H has larger impact than other radicals on combustion characteristics due to its large diffusivity and suppression of a chain branching reaction (H+O\(_2=\)O+OH).

4. Conclusion

Two-dimensional H atom distribution of the CH\(_4\)/air premixed flame in a narrow channel is successfully measured with a newly-developed TALIF setup having high efficiency 205 nm laser. Based on the measured H atom concentration near the wall, a wall radical quenching model focused on H adsorption is proposed and the initial sticking coefficient of H on SUS321 and quartz surfaces are estimated as 0.1 and 0.01, respectively. Sensitivity analysis shows that the H adsorption should be dominant in the wall chemical effect.

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Figure 5. CO and HRR in cases of H, OH, O, CH\(_3\) adsorptions and single radical adsorption.

Figure 6. Effect of H-adsorption. (a) H contours (Inert), (b) H contours (Active), and (c) wall normal distributions of H, OH, O.