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Flame base structures of micro-jet hydrogen/methane diffusion flames

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Abstract

In this study, a comparison of flame base structures of hydrogen/methane–air diffusion flames formed over a tiny-jet is made numerically for both isothermal and thermal conductive burner conditions, in order to clarify the fuel dependent flame stabilization mechanisms. It is found that, unlike a methane flame, the flame base of a hydrogen flame always attaches to the burner. The analyses indicate that the dominant intermediate-consumption steps have significantly lower activation energies for the hydrogen flame as compared to a methane flame. More importantly, one of the HO_2 production reactions (R43f: $H + O_2 + M \rightarrow HO_2 + M$), which has a dominant role in sustaining reactivity at the flame base, shows a negative temperature dependence, causing the heat release rate in the flame base kernel to increase as the burner wall temperature decreases. With a thermal conductive burner (thermal conductivity of 16 W/m-K) over a wide range of fuel jet velocities (0.5–4.0 m/s), it is found that the burner tip is heated to a significantly higher temperature by a hydrogen flame due to its unique stabilization mechanism. The mixing effects of hydrogen and methane are then considered. It is found that the burner tip temperature can be reduced by adding methane into the fuel flow. This is because, according to the investigation of the structures of the hydrogen/methane jet diffusion flames, the reaction rate of R43f is suppressed due to the included intermediates (e.g., CH_3, CH_2O) consumption steps of methane. It is expected that the flame attachment feature associated with the flame base structure can be easily controlled by mixing hydrogen and methane, making it possible to control the burner tip temperature in advance.

Keywords: Micro flame; Extinction; Jet diffusion flame; Hydrogen flame; Flame-burner interaction

1. Introduction

Given that hydrocarbon and oxygenated hydrocarbon fuels have much higher specific energy densities than batteries (e.g., lithium ion batteries) [1], development of *combustion* based micro scale power generation systems (such as micro scale engines and turbines) are especially favored to meet the increasing demands for portable power generators, micro-satellite thrusters, micro unmanned aircrafts, micro reactors, micro sensors, and others. In order to design a compact, stable, and long life combustor or burner for those devices, a deep understanding of the fundamentals of micro scale

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combustion is essential. Both premixed and diffusion combustion strategies should be potential options to utilize thermal energy, while according to the recent reviews [2,3] studies regarding micro diffusion flames are relatively less compared with those for premixed flames.

The micro jet diffusion flame was first studied by Ban et al. [4] about twenty years ago. Fuel was ejected into a quiescent air environment through a submillimeter-diameter burner. Such a tiny flame is stabilized by the burner, and controlled by diffusion and convection whilst the buoyancy effect is minor. Additionally, due to the "inherent" large surface to volume ratio (S/V) feature in miniaturization, flame-burner interaction plays a significant role in the stability of the microflames. For this reason, the stabilization mechanism of micro-jet diffusion flames has been studied by numerous researchers [5–17]. In general, local extinction occurs in the vicinity of the burner wall, and hence there exists a gap (flame quenching zone) between the flame base and the burner wall, as observed in the experiments by Cheng et al. [8,10,11], Kuwana et al. [13] and Fujiwara et al. [14] and Fujiwara and Nakamura [15] for methane flames. Such a gap has been also clearly observed in micro-jet diffusion flames for general carbon-contained fuels, such as ethane, ethylene, and acetylene [4], propane [5], and ethanol [17].

On the contrary, as notified in the previous studies by Cheng et al. [6,9] and our recent numerical work [16] using hydrogen as the fuel, it seems that a hydrogen diffusion flame readily attaches to the burner wall and local extinction may not occur in the vicinity of the burner wall, invoking that the stabilization mechanism for a hydrogen flame may differ from that of a methane flame. Once the flame is fully attached to the burner, substantial heat can be transported (recirculated) to the fuel to improve the flame stability. On the other hand, the burner tip temperature can increase dramatically, causing structural damage (thermal damage to burner). In this regard, a strategy to control the flame base structure (thus the burner tip temperature) is important, especially for microflame technology.

The objective of this study is to clarify the stabilization mechanism of micro-jet hydrogen/methane diffusion flames by numerical approaches. Computations are performed by adopting both isothermal and thermal conductive burner wall boundary conditions to understand the effect of burner wall temperature on the flame attachment mechanism. Fuel mixing effects on the flame base structure are also examined and a strategy to control the burner tip temperature and the degree of heat recirculation is suggested.

2. Numerical approach

The numerical method is similar to our recent work [16]. A set of governing equations of mass, momentum, energy and species are solved in a two-dimensional (r–z) cylindrical coordinate by the commercial software FLUENT 14.5 CFD [18] based on the finite volume method (FVM) with the SIMPLE algorithm. Figure 1 illustrates the schematic of the computation domain and boundary conditions. Fuel is ejected into the ambient air through a tube (burner) with an inner diameter of 0.8 mm and an outer diameter of 1.2 mm. The pressure outlet boundary conditions are imposed at the far field boundaries. The burner wall is assumed to be non-slip, and chemically inert (because the recent study by Kizaki et al. [19] has proved that the effects of surface quenching reactions are minor at normal pressure; catalytic surface reaction assisted diffusion flames could be our future work however it is not considered in this study). Two kinds of thermal boundary conditions are considered at the burner wall. For the isothermal burner conditions, the inner surface and the top surface of the burner wall are assumed to be adiabatic, while the outer surface is set to a temperature of T_b, which varies from 300 K to 1800 K, because in reality a flame shall attach (if it can) to the outer surface of the burner wall, and therefore the outer surface temperature is critical for the flame-burner attachment. For the thermal conductive burner conditions, grid is put in the burner (solid) zone, namely, the thermal conduction equation in the burner zone (solid) is solved as well. Conjugate thermal boundaries are set at the inner surface, the outer surface and the top surface of the wall, while 300 K is imposed at the bottom of the burner wall to allow the heat loss from the domain. Although radiation may more or less affect flame temperatures at near extinction conditions, it has been shown that [8,9] the micro-jet diffusion flame structures could be predicted satisfactorily by the numerical models excluding radiation heat loss. Thus, radiation effects are also

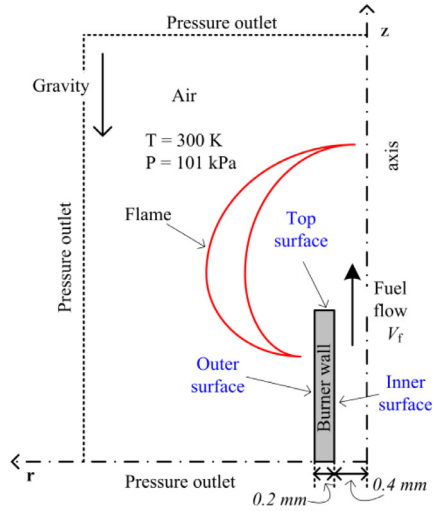

Fig. 1. Schematic of computation domain and boundary conditions.

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