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A numerical study of the auto-ignited laminar lifted methane/hydrogen mixtures in heated co-flow air

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Abstract

In the present study, the liftoff characteristics of a laminar HCNG flame are investigated using 2-D numerical simulations by varying the fuel jet velocity. It is observed that the liftoff height decreases with increasing fuel jet velocity. Gradual transition from the tribrachial flame to the MILD combustion is also observed. From both *Da* analysis and transport budget analysis, it is verified that auto-ignition is the main stabilization mechanism of the lifted flame. Additional simulations are carried out with modified hydrogen diffusivity, showing that the decrease of liftoff height is mainly attributed to the high diffusivity of hydrogen molecule. Preferential diffusion effect of hydrogen is clarified by revising the ignition delay time term in the liftoff height relation. It is also shown that the revised ignition delay time increases as the fuel jet velocity decreases since hydrogen ratio R_H decreases at the upstream of flame front with decreasing fuel jet velocity. The high diffusive nature of hydrogen molecule increases the ignition delay time at lower fuel jet velocity, which, in turn, leads to the increase of the liftoff height.

1 Introduction

With increasing demand of reducing pollutant emissions, compressed natural gas (CNG) is regarded as a suitable fuel to replace other fossil fuels because natural gas is abundant in the world and produces less pollutant emissions. However, it is limited to apply CNG to practical engine systems due to its low ignitability. In this regard, hydrogen addition to the natural gas, known as HCNG or H_2CNG, is highlighted to cope with the limitation of methane combustion based on the hydrogen's high flame speed and wide flammability range [1]. Especially, auto-ignition characteristics of methane/hydrogen mixture plays an important role for the ignition processes in diesel engines. In this study, therefore, the characteristics of auto-ignited laminar lifted flames of HCNG in heated co-flow jets are numerically investigated.

According to the previous experimental study, auto-ignited laminar fuel is stabilized either lifted flame or nozzle attached flame shape depending on the initial conditions, and lifted laminar jet flame is categorized into tribrachial flame and MILD combustion regimes [2,3]. Adiabatic ignition delay time is identified as one of the key factors for the stabilization of auto-ignited lifted flame, and the liftoff height relation $H_L \sim U_0 t_{\mathrm{ig,ad}}^2$ is derived and correlated well with the various fuels for the tribrachial flames, where H_L is the liftoff height, U_0 is the fuel jet velocity, and $t_{\mathrm{ig,ad}}$ is the adiabatic ignition delay time at the stoichiometry condition. Therefore, the liftoff height H_L generally increases with increasing U_0 since $t_{\mathrm{ig,ad}}$ has nothing to do with U_0.

In the auto-ignition of HCNG, however, an unusual phenomenon was observed from previous experiment [4] that liftoff height H_L decreases with increasing jet velocity U_0 at relatively low temperature. This behavior was not observed previously, and the reason was not fully understood yet. Note that when initial concentration of hydrogen is relatively low, the methane/hydrogen mixture exhibits the conventional lifted jet flame characteristics such that liftoff height increases with increasing fuel jet velocity. We can observe the unusual decreasing behavior above only when the amount of hydrogen in fuel jet is relatively high. The exact hydrogen ratio level leading to the decreasing liftoff height behavior highly depends on the initial co-flow temperature.

Another unique characteristic of the auto-ignition of HCNG in laminar co-flow jet is that transition from tribrachial flame to MILD combustion occurs when U_0 becomes low enough even though fuel mole fraction in fuel jet is the same.

The purpose of the present study, therefore, is divided into three parts: (1) understanding the stabilization mechanism of HCNG auto-ignited lifted flame, (2) clarifying the decreasing behavior of H_L with increasing U_0, and (3) elucidating the MILD combustion characteristics of HCNG lifted flame.

2 Numerical methods

Two-dimensional numerical simulations are performed using laminarSMOKE [5,6], which is an OpenFOAM based laminar reacting flow solver. The laminarSMOKE code is a numerical framework for the simulation of laminar flames in multi-dimensional geometries with detailed kinetics. The conservation equations of mass, momentum, species, and energy are solved.

In the present study, a skeletal methane-air kinetic mechanism of 30 species and 184 reactions is used [7]. Following the

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previous experimental setup [2~4], an axisymmetric domain of 6.65 cm × 30 cm in the r- and z-directions is adopted. In the r-direction, a 100 μm mesh is uniformly distributed within 1 cm, and stretched mesh is applied to the remaining area. In the z-direction, a uniform grid of 100 μm is used. Inlet temperature, T_0, for both fuel jet and coflow is 950 K and jet velocity, U_0, varies from 3 to 25 m/s. Fuel mole fraction at fuel jet, $X_{F,0}$, is 0.2, and the hydrogen ratio in the fuel jet, R_H, is 0.3.

A grid convergence test is carried out for the case with U_0 = 15 m/s. The results show that the present grid size of 100 μm is fine enough to capture the flame structure and predict the liftoff height well compared to those with a finer grid size. Hence, all of the simulations in the present study use the grid system of 100 μm.

3 Results

3.1 General characteristics of lifted flame

Figure 1 shows temperature isocontours for the auto-ignited HCNG lifted flames with various jet velocities. As shown in the figure, the present simulation results can capture the unique characteristic of HCNG combustion that the liftoff height decreases with increasing jet velocity. Here, the flamebase is defined as the lowest z position of λ_{exp}= 0 iso-contour. Note that λ_{exp} is an eigenvalue of the Jacobian, J_w, of the chemical source term ω in a reacting governing equation. For the details of λ_{exp}, readers are referred to [8~]. The point where λ_{exp} crosses zero is defined as a 'crossover point' between non-explosive and explosive regions and it can be used to detect the flamebase, especially for lean mixtures.

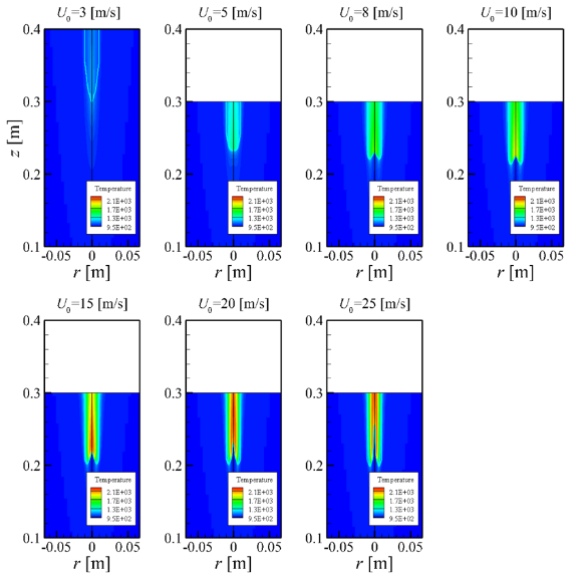

Figure 1: Temperature isocontours with various fuel jet velocities

For cases with relatively low U_0 (equal to or less than 5 m/s), the lifted flames do not feature the typical tribrachial lifted flame shape. This is because they can be categorized into the moderate or intense-low oxygen dilution (MILD) combustion regime, where the conditions of $(T_{max} - T_0)/T_{ig} < 1$ and of $T_{max} > 1$ are both satisfied.

Figure 2 shows the liftoff height as a function of fuel jet velocity and the corresponding temperature index to determine MILD combustion condition. Two points are noted from the figure. First, as reported in a previous experimental study [4], the liftoff height decreases with increasing U_0, which is an unusual feature of lifted flame behavior. Second, the liftoff height increases significantly under the MILD combustion regime, which will be discussed in the following section.

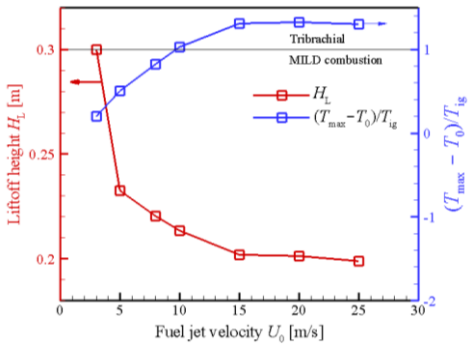

Figure 2: Temperature and temperature index with various fuel jet velocities.

3.2 Flame stabilization mechanism

To understand the unique phenomena of auto-ignited HCNG lifted flames, their flame stabilization mechanism is first elucidated. In the present study, both Damköhler number and transport budget analyses are carried out for all cases to demonstrate how auto-ignition or flame propagation affects the stabilization of the flamebase.

Damköhler number, $\boldsymbol{Da}$, is defined as the ratio of the characteristic flow time to the characteristic ignition delay time, $\boldsymbol{Da = t_{flow}/t_{ig}}$. It is evaluated at every single point in a streamline which passes through the flamebase. The characteristic flow time, $\boldsymbol{t_{flow}}$, is defined as the required time for a fluid particle to arrive at the flamebase starting from each point in the streamline. The characteristic ignition time, $\boldsymbol{t_{ig}}$ is the 0-D ignition delay time at each point. Therefore, when $\boldsymbol{Da > 1}$ region exists at the upstream of flame base, $\boldsymbol{t_{ig}}$ is shorter than $\boldsymbol{t_{flow}}$, implying that auto-ignition can occur at the upstream and the flamebase may be stabilized by auto-ignition. On the other hands, if $\boldsymbol{Da < 1}$ along the streamline from the flamebase, $\boldsymbol{t_{ig}}$ is always larger than $\boldsymbol{t_{flow}}$, indicating that auto-ignition may not be dominant upstream of the flame base. Therefore, the flamebase is stabilized by flame propagation rather than auto-ignition.

Figure 3 shows Da along the streamline passing the flamebase for cases with U_0 = 8 and 25 m/s. From the figure, it is readily observed that Da becomes greater than unity at the far upstream of the flamebase, which implies that the lifted flame is stabilized by auto-ignition rather than flame propagation. Similar trend is observed for the other cases (not shown here).

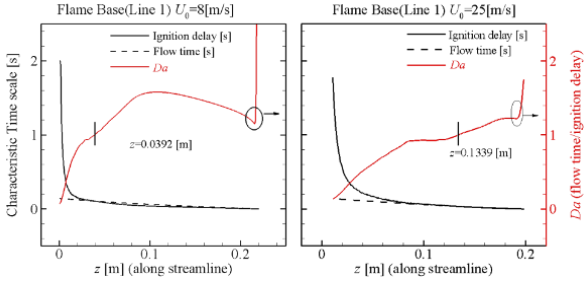

Figure 3: *Da* analysis for cases U_0 = 8 (left) and 25 m/s (right).

To further identify the stabilization mechanism of the lifted flames, the transport budget analysis is also performed along the streamline passing through the flamebase. Species transport equation for the given species *i* is given by:

$$\frac{\partial(\rho Y_i)}{\partial t} = -\frac{\partial(\rho Y_i u_j)}{\partial x_j} - \frac{\partial(\rho Y_i V_{j,i})}{\partial x_j} + \omega_i, \qquad (1)$$

where ρ is density, Y_i is species mass fraction, $V_{j,i}$ is the diffusion velocity, and ω_i is the species mass reaction rates. The left hand side of Eq. (1) is zero since all of simulations reaches the steady state. The first term on the right hand side indicates the convection, the second term represents diffusion, and the last term is reaction. Each term for OH species is evaluated along the streamline. As in the *Da* analysis, cases with U_0 = 8 and 25 m/s are analyzed and the other cases show similar results. As shown in Fig. 4, the convection term balances reactions term and the diffusion term is relatively small compared to the other terms, verifying that the flamebase is stabilized by auto-ignition rather than flame propagation.

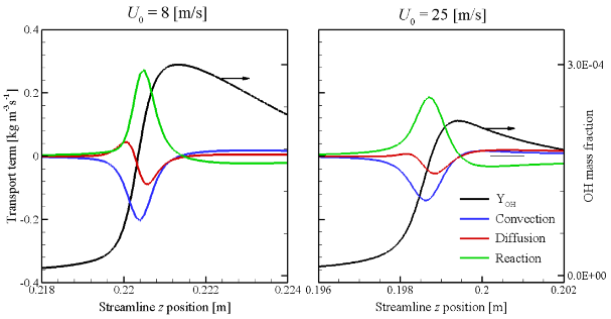

Figure 4: Budget analysis of OH species transport equation and OH mass fraction along the streamline.

3.3 Decreasing behavior of H_L

In the previous experiment [4], it was conjectured that the differential diffusion of the duel fuel, especially the high mass diffusivity of hydrogen, would be primarily attributed to the decrease of the liftoff height with increasing U_0. To verify the effect of hydrogen molecule's high diffusivity on the lifteoff height, additional numerical simulations are performed by setting the mass diffusivity of hydrogen molecule to that of methane. Figure 5 shows the liftoff height and temperature index $(T_{max} - T_0)/T_{ig}$ for cases with real and modified diffusivity of H_2. Except for the MILD combustion regime, modified diffusivity cases show that the liftoff height increases with increasing jet velocity, which follows the conventional liftoff height tendency. This result proves that the high diffusive nature of hydrogen molecule is attributed to the decrease of H_L with increasing U_0. To incorporate the effect of large mass diffusivity of H_2 into the liftoff height model, $H_L \sim U_0 t_{ig,ad}^2$, we come up with a modified ignition delay time. The adiabatic ignition delay time, $t_{ig,ad}$, corresponds to the 0-D ignition delay time of the stoichiometric mixture of fuel jet and coflow air, and hence, the differential diffusion effect of the dual fuel cannot be accounted for in the liftoff height relation. For auto-ignition of single fuel jets such as methane or propane, the conventional liftoff height relation is well correlated with both experimental and numerical results. For dual fuel jets such as HCNG, however, the ignition delay time cannot be determined solely from the fuel jet composition because the hydrogen content varies significantly depending on the location of the flamebase. In this study, the modified ignition delay time, t_{ig}, is obtained by tracing the

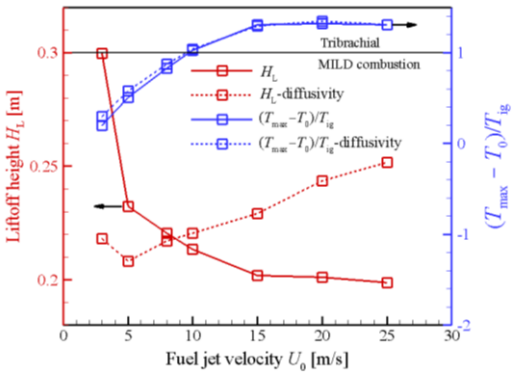

Figure 5: Temperature and temperature index with various fuel jet velocities for both real and modified diffusivity of H_2. Solid line is real, dashed line is modified H_2 diffusivity cases.

initial mixture composition of the flamebase. Based on the mixture contents at the flame base, we can find the mole fraction of initial mixture composition: CH_4, H_2, O_2, and N_2 (referred to hereinafter as 'evaluated initial mixture composition'). Our assumption is that 0-D ignition delay time of evaluated initial mixture composition would represent the characteristic ignition delay time in 2-D domain since it includes the information on the different diffusion effect led by different convection time scale.

Figure 6 shows the modified liftoff height relation $H_L \sim U_0 t_{ig}^2$ and actual liftoff height H_L. It is readily observed from the figure that the modified liftoff height relation is well correlated with both real and modified H_2 diffusivity cases. Note that to find H_L correlation, we divide it into two regimes: tribrachial flame regime and MILD combustion regime.

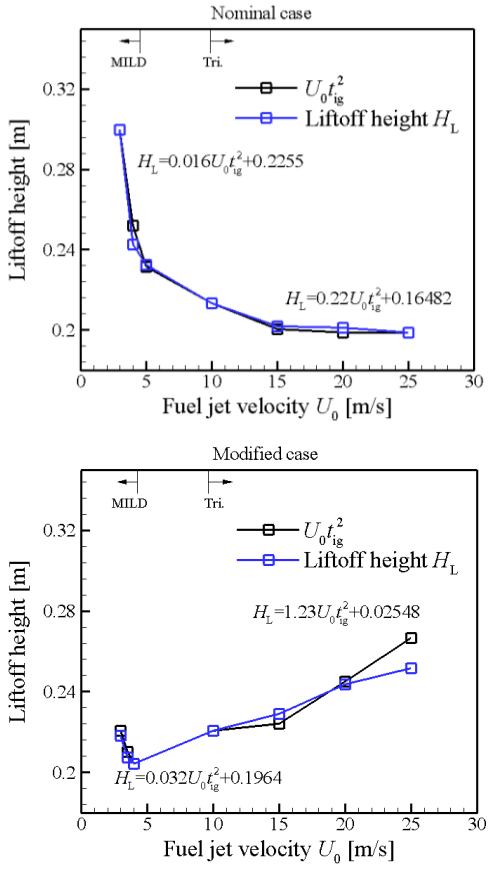

Figure 6: The relationship between $H_L \sim U_0 t_{\mathrm{ig,ad}}^2$ and actual liftoff height H_L for real (above) and modified H_2 diffusivity cases (below).

Figure 7 shows the modified ignition delay time, t_{ig}, and hydrogen ratio, R_{H}, with various jet velocities. R_{H} is obtained from the evaluated initial mixture composition. It is readily observed from the figure that t_{ig} decreases as U_0 increases. It is of importance to note that t_{ig} significantly increases under the MILD combustion conditions compared to the tribrachial conditions. This is because under the MILD combustion conditions, the flamebase is located at the centerline and the corresponding hydrogen content vanishes there. As shown in Fig. 8, the more hydrogen molecules are included in the mixture or the higher R_{H} is, the shorter the ignition delay time is.

In summary, under the tribrachial flame conditions, hydrogen molecules can diffuse out more radially with increasing U_0, and subsequently, the R_{H} at the flamebase increases, leading to the shorter H_L. Under the MILD combustion conditions, the R_{H} vanishes at the flamebase and hence, the ignition delay time is increased, resulting in the longer H_L. Under either conditions, the large mass diffusivity of hydrogen molecule together with the flamebase location is primarily attributed to the decrease of H_L with increasing U_0.

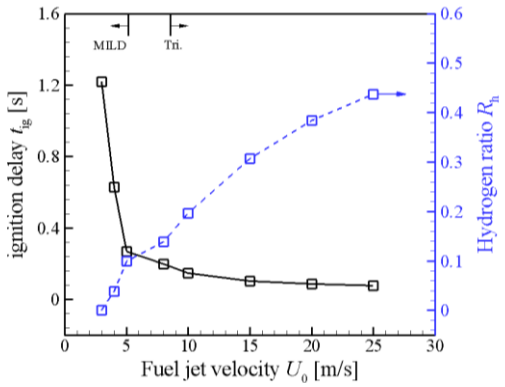

Figure 7: 2-D ignition delay time (black solid) and hydrogen ratio R_{H} at the flame base (blue dotted) with the different fuel jet velocities.

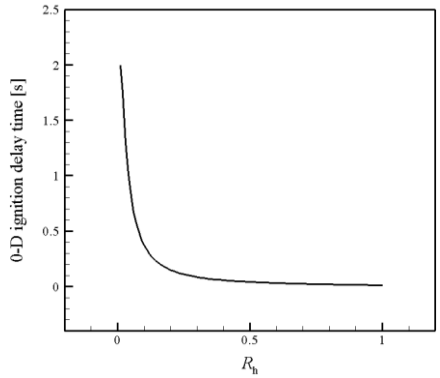

Figure 8: 0-D ignition delay time as a function of the hydrogen ratio R_{H}. Initial temperature for the 0-D calculation is 950 K, and pressure is 1 atm. Fuel mole fraction of the fuel jet $X_{F,0}$ is 0.2.

Although it is not shown in the present paper, additional numerical simulations were carried out with the initial condition of $T_0 = 1000$ K and $R_{\mathrm{H}} = 0.08$ in fuel jet. The result revealed that the liftoff height is proportional to the fuel jet velocity. It is consistent with the previous experimental results, which showed that liftoff height change trend in HCNG is sensitive to the both initial temperature and hydrogen concentration level in fuel jet.

4 Conclusions

The conclusions of the present study are as follows.

(1) From the *Da* analysis and transport budget analysis, it is found that the lifted flames are stabilized by auto-ignition rather than flame propagation. Therefore, ignition delay time, $t_{\mathrm{ig,ad}}$, plays a key role in determining the liftoff height.

(2) The large diffusivity of hydrogen molecule is the main factor to induce the unusual tendency of the liftoff height; H_L decreases as U_0 increases. Depending on U_0, the lifted flames belong to either tribrachial flame or MILD combustion. As such, we could obtain two different H_L correlations corresponding to the tribrachial and MILD combustion regimes. This is because the ignition delay time changes significantly under the MILD combustion conditions (lower R_{H}), whereas it marginally varies under the tribrachial flame conditions (higher R_{H}).

(3) The MILD combustion in HCNG occurs when U_0 is relatively low. As the jet velocity becomes low, the hydrogen molecules in the fuel jet are more apt to diffuse out radially and finally the content of hydrogen vanishes at the flamebase. As a result, the ignition of the fuel jet is more delayed and the fuel mole fraction at the flamebase decreases significantly, leading to the combustion mode change from the tribrachical flame to the MILD combustion.

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