A Comparative DNS Study of Turbulent Lifted Hydrogen/Air Jet Flame near Auto-Ignition Limit

Seung Ook Kim[1], Jacqueline H. Chen[2], and Chun Sang Yoo[1, *]

[*]Corresponding author: csyoo@unist.ac.kr

[1]School of Mechanical and Nuclear Engineering, Ulsan National Institute of Science and Technology, Ulsan 689-798, Republic of Korea

[2]Combustion Research Facility, Sandia National Laboratories, Livermore, CA94551-0969, USA

Introduction

The characteristics of turbulent non-premixed lifted jet flames under various coflow conditions have widely been investigated due to their relevance to practical applications such as diesel engines, gas turbine combustors, and commercial boilers. Moreover, the stabilization mechanisms of turbulent lifted jet flames are so complicated that it is still challenging to develop a predictive model, which is able to describe correctly every situation in turbulent combustion. In such modern combustion systems, fuel is usually injected into an environment of hot gases such that turbulent flames may be stabilized through the recirculation of hot air and combustion products. Under such conditions, this leads to a turbulent lifted flame, and the hot environment admits the possibility of auto-ignition as a mechanism contributing to the stabilization of the flame base. In addition to auto-ignition, flame propagation and the role of large eddies have been considered as possible mechanisms for stabilization of the lifted flame base[1,2]. In our previous 3-D direct numerical simulation (DNS) study of turbulent lifted jet flames in autoignitive coflows, it was found that the lifted flame base forms a cycle with the passage of large-scale jet structure and the stabilization is determined by the competition between local axial velocity and auto-ignition that occurs in fuel-lean mixtures[1,2]. We have recently performed three 3-D DNSs of a turbulent lifted hydrogen/air jet flames in heated coflows near auto-ignition limit to examine the stabilization mechanisms and flame structure of turbulent lifted jet flames.

Problem configuration

The spatially-developing turbulent lifted jet flame simulation was performed in a 3-D slot-burner configuration. Fuel issues from a central jet, which consists of 65% hydrogen and 35% nitrogen by volume at an inlet temperature of T_j = 400K. The central jet is surrounded on either side by co-flowing heated air streams at three different T_c = 750 (Case L), 850 (Case M), and 950 K (Case H) and atmospheric pressure. The fuel jet and coflow velocities are specified as U_j = 240 m/s and U_c = 2 m/s, and the fuel jet width, H, is 2 mm such that the jet Reynolds number, Re_j (= HU_j/ν), is approximately 8,000. The computational domain is $15H \times 20H \times 3H$ in the streamwise, x, transverse, y, and spanwise, z, directions with $2000 \times 1600 \times 400$ grid points. A uniform grid spacing of 15 μm is used in the x- and z-directions, while an algebraically stretched mesh is used in the y-direction.

The compressible Navier-Stokes, species continuity, and total energy equations were solved using the Sandia DNS code, S3D, with a 4th-order Runge-Kutta method for time integration and an 8th-order central differencing scheme for spatial discretization. A detailed hydrogen/air kinetic mechanism was adopted for DNSs[3]. Improved nonreflecting inflow/outflow boundary conditions[4] were used in the x- and y-directions and periodic boundary conditions were applied in the homogeneous z-direction. Based on the fuel jet velocity and the streamwise domain length, a jet time, $\tau_j = L_x/U_j$, is approximately 0.125 ms. To obtain a stationary lifted flame while saving computational cost, a simulation with a grid resoution of 40 μm was first performed until the flame reached a steady state. The solution from that simulation was then interpolated to 15 μm and used as an initial condition for the fully resolved simulation. The solution was advanced at a constant time-step of 5 ns through 4.0 τ_j. The fine-mesh simulations were performed on the Cray XT5/XK7 at Oak Ridge National Laboratories and each DNS required 2.5 million CPU-hours. Note that the steady lift-off heights are approximately $\bar{h}_L/H = 2.4$, $\bar{h}_M/H = 4.0$, and $\bar{h}_H/H = 5.3$.

Results and Discussion

Figure 1 shows 3D volume rendering of OH and HO_2 mass fractions, and 2D isocontour of Damköhler number, Da, for the three cases. $Da = \lambda_e \cdot \chi^{-1}$ where χ is the scalar dissipation rate and λ_e is a chemical mode which is an eigenvale of the Jacobian matrix of chemical source term in the governing equations. A chemical explosive mode (CEM) is defined as the chemical mode of which λ_e is positive. In general, a mixture with $Da \gg 1$ is likely to lead to ignition, and as such, a long strip of mixture with large Da upstream of the flamebase in Case H indicates that auto-ignition by high coflow temperature can be the main source of the flame stabiliztion for Case H. For Cases L and M,

however, only a narrow tip of mixture with large Da upstream of the flamebases exists, which indicates that flame propagation rather than auto-ignition can be attributed to the stabilization of the lifted flame even for Case M with the coflow temperature being close to auto-ignition limit. Note that usually, Da has large value in the preheating zone of a premixed flame such that the narrow regions with large Da in Case L and M are the preheating zone and not the radical-induced ignition[5,6].

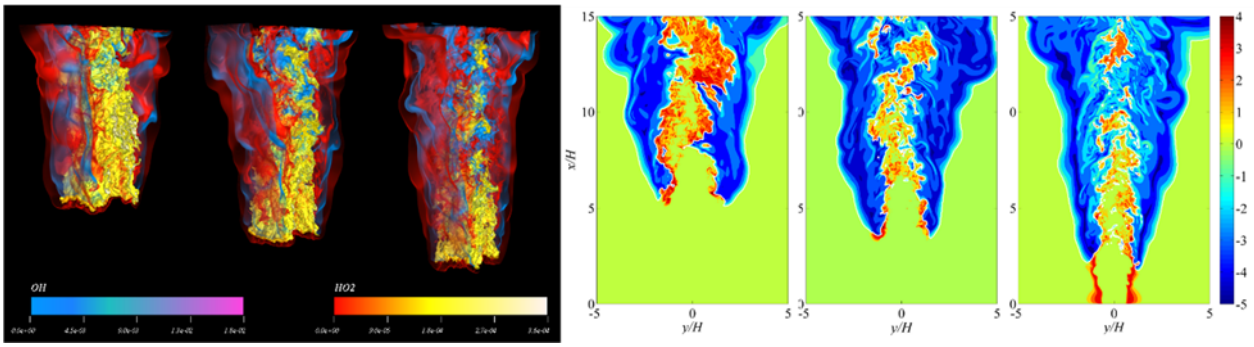
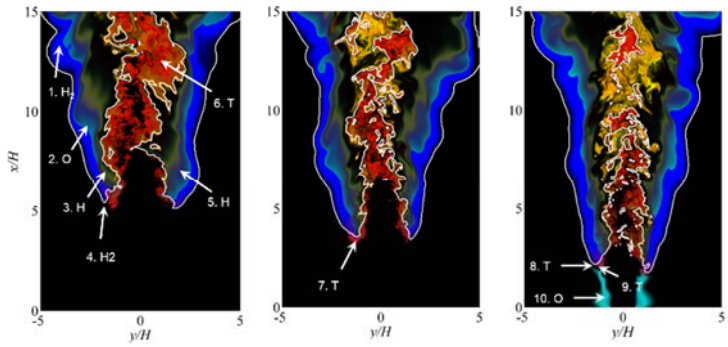


Figure 1. 3-D volume rendering of OH and HO_2 mass fractions, and isocontours of Da (log scale) for Cases L, M, and H (from left to right). White lines denote the flamebase with $Da = 1$.

The physicochemical characteristics of the flames are further investigated using the explosion index (EI) and participation index (PI), which represent the contribution of a chemical species and a reaction to a CEM, respectively. Especially, the EI's and PI's at ten different locations are listed in the table. It is of interest to note that temperature and hydrogen are the most important species at right upstream of the flamebases for all cases regardless of the coflow temperature, and R1 ($H + O_2 = O + OH$) and R9 ($H + O_2 + M = HO_2 + M$) are the two major reaction steps, contributing to the CEM.



Points	Location	EI, Species	PI, Reactions
1	x=13.18H y=-4.03H	0.99, H_2	0.49, R3: $H_2 + OH = H_2O + OH$ 0.13, R9: $H + O_2 + M = HO_2 + M$
2	x=9.24H y=-2.61H	0.40, O 0.27, H	0.69, R9: $H + O_2 + M = HO_2 + M$ 0.14, R8: $H + OH + M = H_2O + M$
3	x=6.90H y=-1.71H	0.56, H 0.19, O_2	0.70, R8: $H + OH + M = H_2O + M$
4	x=5.34H y=-1.8H	0.49, H_2 0.47, T	0.49, R1: $H + O_2 = O + OH$ 0.43, R9: $H + O_2 + M = HO_2 + M$
5	x=6.96H y=2.01H	0.37, H 0.28, H_2	0.67, R8: $H + OH + M = H_2O + M$ 0.18, R9: $H + O_2 + M = HO_2 + M$
6	x=12.48H y=1.05H	0.84, T	0.34, R11: $HO_2 + H = OH + OH$ 0.19, R3: $H_2 + OH = H_2O + OH$
7	x=3.33H y=-1.26H	0.87, T	0.43, R9: $H + O_2 + M = HO_2 + M$ 0.38, R1: $H + O_2 = O + OH$
8	x=2.13H y=-1.47H	0.53, T 0.41, H_2	0.50, R9: $H + O_2 + M = HO_2 + M$ 0.50, R1: $H + O_2 = O + OH$
9	x=2.04H y=-1.23H	0.69, T 0.15, H_2	0.48, R9: $H + O_2 + M = HO_2 + M$ 0.47, R1: $H + O_2 = O + OH$
10	X=-0.93H Y=0.54H	0.80, O 0.18, OH	0.40, R1: $H + O_2 = O + OH$ 0.40, R9: $H + O_2 + M = HO_2 + M$

Figure 2. EI-weighted color-mixing of temperature (red), H_2 (blue), H (green), O (cyan), O_2 (yellow) for Cases L, M, and L from left to right, and EI and PI at selected points (see table) .

The Favre means and variances of temperature, heat release, Da, and important species are evaluated at different axial locations, all of which show the flame propagation or auto-ignition characteristics depending on the coflow temperature.

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