

Effect of steam dilution level on partially premixed lifted flame

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Direct numerical simulations (DNS) have been performed for laminar hydrogen-oxygen lifted flame at elevated pressure. The DNS is parametrized by composition, diluent, temperature and pressure conditions with focusing on next generation high diluted hydrogen gas turbine at elevated pressure to investigate their effects on the overall flame structure in the mixture fraction space and interactions between triple flame branches. It is observed that the flame base is relatively thinner in upstream, which thickens with the transverse distance for non-steam dilution cases. For high pressure steam diluted cases, the flame is observed as a thin flame consisting of double branches structure with annihilation of the lean branch.

1. Introduction

In recent years, hydrogen combustion technology started to attract many companies to represent the next generation of power plants combustor. However, hydrogen combustion has a problem of producing high temperature which would lead to NO_x formation causing environmental issues. Moreover, it causes flame control problems and combustion instability. One of the approaches to address this issue is to use pure oxygen for hydrogen combustion, instead of the air, which includes nitrogen. However, this approach increases the combustion temperature significantly, hence the material components consisting the combustor cannot withstand under that severe temperature condition. To give promising solution to avoid this high temperature problem and to achieve stable combustion, dilution of hydrogen/oxygen with steam and preheating have been proposed in this research.

A lifted jet flame has several practical applications such as primary combustion zones in staged gas-turbines for power generation, reburn zones in utility boilers, and many industrial burners. Several numerical and experimental studies have been conducted to understand the leading-edge flame structure as reviewed by Buckmaster, 2002⁽¹⁾, and they observed the triple flame structure which is located around the stoichiometric line, where the non-premixed flame exist bounded by two lean and rich premixed flame branches in the oxidizer and fuel side respectively.

Various studies have also focused on jet flame stabilization mechanism based on different theories of (premixedness, large eddies and critical dissipation rate concept). Premixedness stabilization mechanism, which is originally proposed by Buckmaster and Weber 1996⁽²⁾, is based on the upstream edge flame propagation speed along the stoichiometric line with relative to the inflow speed. The role of large structures eddies on the stabilization mechanism was also reported by Dahm and Mungal, 1985⁽³⁾ that the large structure produces pockets of hot burned products, which is transported in the upstream direction and reignite the fresh fuel and oxidizer. Miake-Lye and Hammer 1989⁽⁴⁾ proposed a different mechanism that is based on the critical dissipation rate, in which the flame moves upstream until the strain rate exceeds the critical value and the flame moves downstream again.

However, there are few studies have been carried out considering highly diluted and preheated mixtures, which is relevant to the next generation high diluted gas turbine condition. Such an extreme dilution condition could influence overall lifted flame structure, similar to which has been reported for extreme DME mixtures, 2015⁽⁵⁾, thereby affecting the lifted flame stabilization and its mechanisms. Thus, it is important to understand the effects of thermo-chemical condition on the flame structure.

The objective of this study is to investigate the effect of steam dilution on the lifted jet flame structure. Four direct numerical simulation cases are performed laminar flames at different thermochemical conditions including at elevated pressure with high dilution conditions. The flame structure is discussed and comparing with the conventional structure based on the direct numerical simulation results.

2. Direct Numerical Simulations

The DNS have been performed using TTX solver developed at Tokyo Institute of Technology⁽⁶⁻⁸⁾. TTX solves the fully-compressible conservation equations for mass, momentum, energy and species mass fraction considering temperature dependent transport properties on Cartesian mesh. The spatial derivatives are approximated using a fourth-order central difference scheme, which gradually changes to a fourth-order one sided scheme near the computational boundaries. The time integration is implemented using the third order Runge-Kutta scheme. In addition, split method with multi-time scale (MTS) solver and correlated dynamic adaptive chemistry and transport (CODACT) are applied for the time integrations of chemical source terms in species conservation equations to reduce the computation time⁽⁹⁻¹¹⁾. Navier-Stokes characteristic boundary condition (NSCBC)^(12, 13) is imposed on the boundaries to prevent artificial pressure reflections. The chemistry is described by detailed kinetic mechanism high pressure by Burke *et al.*, 2011.⁽¹⁴⁾ derived based on that of Li *et al.*⁽¹⁵⁾. The chemical mechanism is comprised of 13 reactive species and 27 elementary reactions is considered to represent hydrogen-air reaction. TTX evaluates reaction rates, thermodynamic and mixture-averaged transport properties based on CHEMKIN II packages^(16, 17).

3. DNS Configuration

The lifted jet flame simulations have been performed in a two-dimensional slot-burner configuration, which is similar to the previous lifted flames DNS performed by Yoo *et al.*, 2009⁽¹⁸⁾ and is presented in Fig. 1a. The following profile is used to specify all the scalars Ψ :

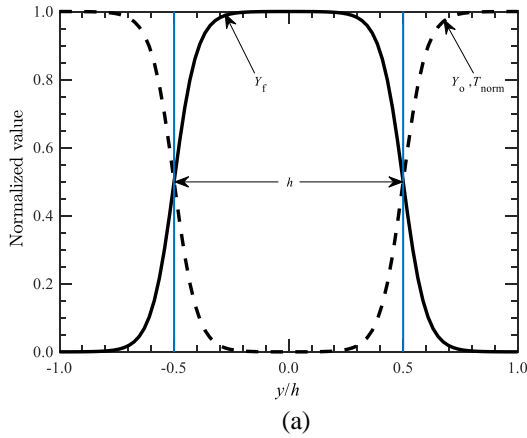
$$\Psi = \Psi_c + \frac{\Psi_i - \Psi_c}{2} \left(\tanh\left(\frac{y+h/2}{2\delta}\right) - \tanh\left(\frac{y-h/2}{2\delta}\right) \right), \quad (1)$$

where h is the jet width at the inlet which has been chosen based on required combustor power with the maximum fuel consumption conditions and δ is specified as momentum layer thickness ($0.05h$). The DNS parameters and thermochemical conditions are presented in Table 1. A fixed, uniform streamwise velocity U_{in} is imposed at the lower (x) boundary, 1995⁽¹⁹⁾. High temperature regions are imposed near the fuel-oxidizer shear layers initially to ignite the mixture, as presented in Fig. 1b. The samples are taken for analysis after solution reaches steady state.

4. Thermochemical Conditions

The simulations have been carried out for 4 different thermochemical conditions as described in Table 1 where stoichiometric mixture fraction was calculated based on Bilger's definition⁽²⁰⁾.

$$\xi = \frac{2Z_C/W_C + \frac{1}{2}Z_H/W_H + (Z_{O,2} - Z_O)/W_O}{2Z_{C,1}/W_C + \frac{1}{2}Z_{H,1}/W_H + Z_{O,2}/W_O}, \quad (2)$$



where Z_j and W_j are the elemental mass fractions and atomic masses for the elements carbon, hydrogen and oxygen and the subscripts 1 and 2 refer to fuel and air streams, respectively. Moreover, for steam cases, to ensure that all steam is injected in a gaseous phase and to avoid any evaporation, additional consideration was taken into account based on Wagner liquid-vapor pressure equation⁽²¹⁾ and the results were verified by experimental results obtained by Kuznetsov, 2011⁽²²⁾.

5. Results and Discussions

General Flame Features

Figure 3 shows the instantaneous temperature fields for the laminar jet flames at different thermochemical conditions after the steady state is achieved in terms of lift of length and flame structure for cases (a, b, c, d), respectively. These results show that the general flame structure are dissimilar for the all cases as follows. The case 1 (Fig. 3a) represents the auto-ignition case due to high T_o (as in Yoo *et al.*, 2009⁽²³⁾), where auto-ignition first occurs around the most reactive mixture fraction (Mastorakos *et al.*, 1997⁽²⁴⁾) followed by the flame development towards downstream. The case 2 (Fig. 3b) the flame is stabilized by propagation due to lower T_o , and overall flame shape shows wider in the transverse direction. The case 3 (Fig. 3c), the steam dilution case, the flame base is wide in the transverse direction, whereas the corresponding dilution case with elevated pressure, case 4 (Fig. 3d), shows the narrow flame base, possibly implying a competing effect of water dilution (wider base) and higher pressure.

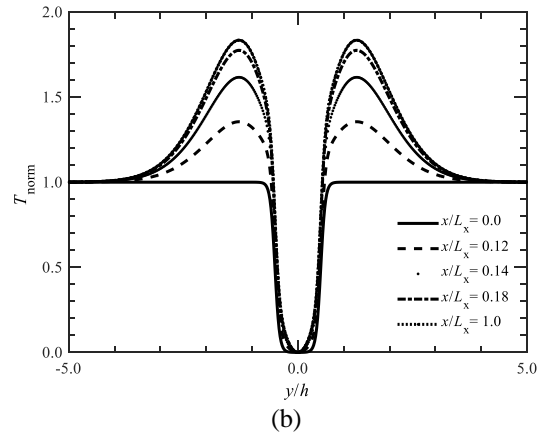


Fig. 1 (a) Mean profile at inlet normalized temperature, blue line represents the inlet jet width (h) where $T_{norm}=(T-T_o)/(T_f-T_o)$. (b) Axial variation of initial normalized temperature.

Table 1. Numerical and physical parameters of the DNS.

	Case 1	Case 2	Case 3	Case 4
Jet width (h)	0.8 mm			
Domain size ($L_x \times L_y$)	32 mm \times 14 mm			
Number of grid points ($N_x \times N_y$)	1800 \times 792	1920 \times 912	1600 \times 720	1800 \times 792
Inlet velocity (U_{in})	35 m/s	12 m/s	1.2 m/s	0.24 m/s
Pressure (P)	1 atm	1 atm	1 atm	10 atm
Fuel Temperature (T_f)	400 K	400 K	288 K	288 K
Oxidizer Temperature (T_o)	1100 K	700 K	870 K	870 K
Fuel Composition (by volume)	35 % H ₂ + 65 % N ₂	H ₂	H ₂	H ₂
Oxidizer Composition (by volume)	Air (21% O ₂ +79%N ₂)	Air (21% O ₂ +79%N ₂)	(0.08% O ₂ +92%H ₂ O)	(8% O ₂ +92%H ₂ O)
Stoichiometric mixture fraction ξ_{st}	0.1993	0.0285	0.1022	0.1022
Laminar flame thickness δ_{th}	0.4756 mm	0.3550 mm	0.7228 mm	0.5015 mm

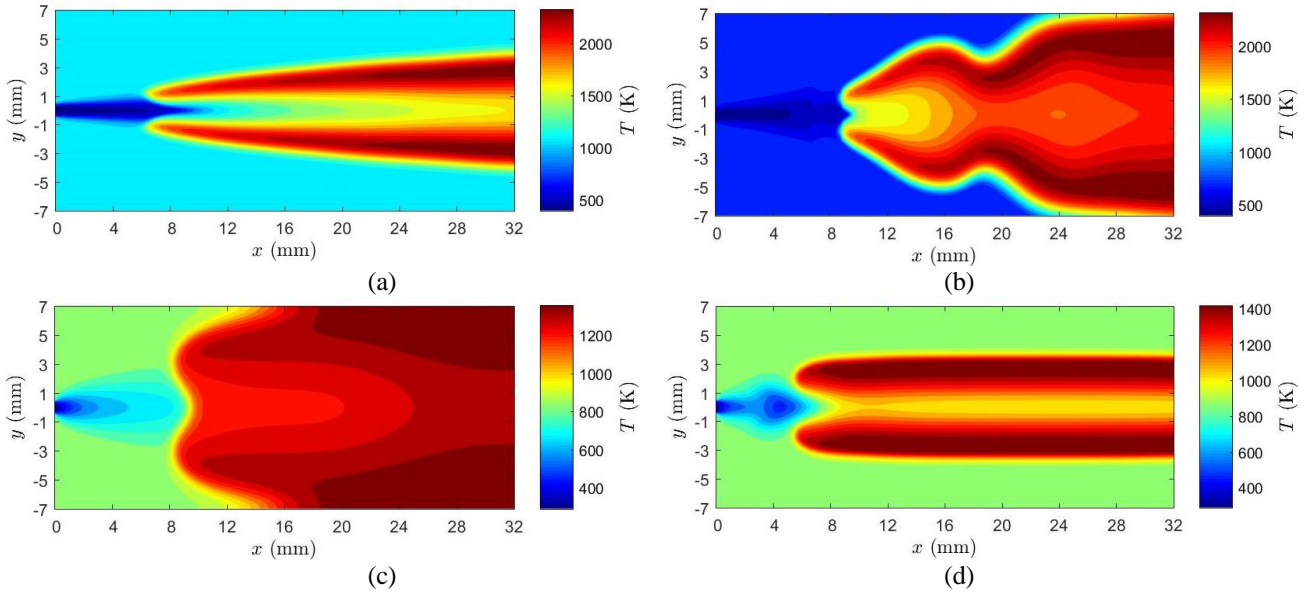


Fig. 3 Temperature fields for laminar jet flames at different thermochemical conditions for case 1 (a), case 2 (b), case 3 (c) and case 4 (d).

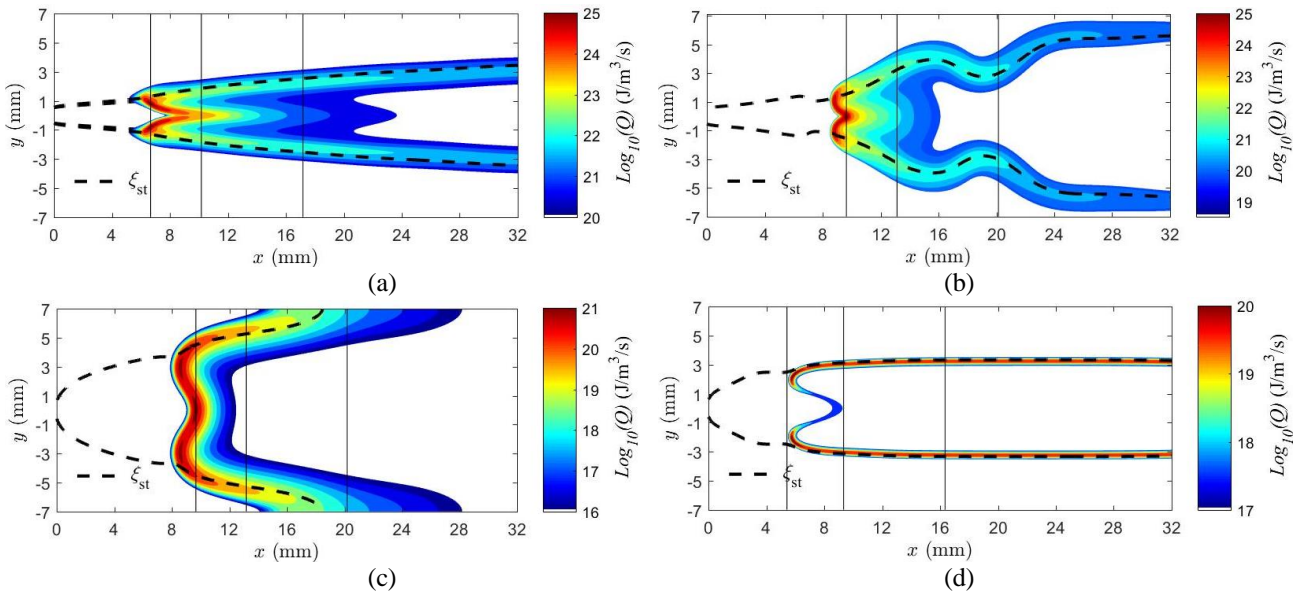


Fig. 4 Logarithmic heat release rate (J/m³/s) field of a laminar flame reported for different cases. Case 1 (a), case 2 (b), case 3 (c) and case 4 (d), dashed line represents stoichiometric line, ζ_{st} and the vertical thin lines indicate sampling locations, x_i .

Flame Structure

Figure 4 shows the logarithmic heat release rate field with the stoichiometric mixture fraction iso-line (ζ_{st}). The figure shows that, for all cases, the flame is evolved around the stoichiometric mixture fraction line. Also, for cases 1, 2 and 3 (Fig. 4a, 4b and 4c), two flame bases are connected via high heat release rate region represented by red color. This is due to the close distance between two “triple flames”, given the relatively narrow jet width compared to corresponding laminar flame thickness. Due to high pressure condition of cased (d) the flame become thinner and similar connection of two flame bases is not observed. Thus, flame base structure depends on the balance between the jet width and inherent laminar flame thickness.

Degree of Mixedness

The flame index has been originally proposed by Yamashita *et al.*, 1996⁽²⁵⁾ to be used to distinguish premixed flames from diffusion flames in turbulent non-premixed jet flames. Using the flame index, Mizobuchi *et al.*, 2002⁽²⁶⁾ observed non-premixed, lean-premixed and rich-premixed flames at the flame base from three-dimensional DNS of a turbulent lifted hydrogen jet flame in a quiescent ambient air. In current two-dimensional DNS of a lifted flame study the normalized flame index FI is used, defined as

$$FI = \nabla Y_F \cdot \nabla Y_O / |\nabla Y_F| |\nabla Y_O|, \quad (3)$$

where Y is the mass fraction, the subscripts F and O denotes represent fuel and oxidizer, respectively. The FI represents

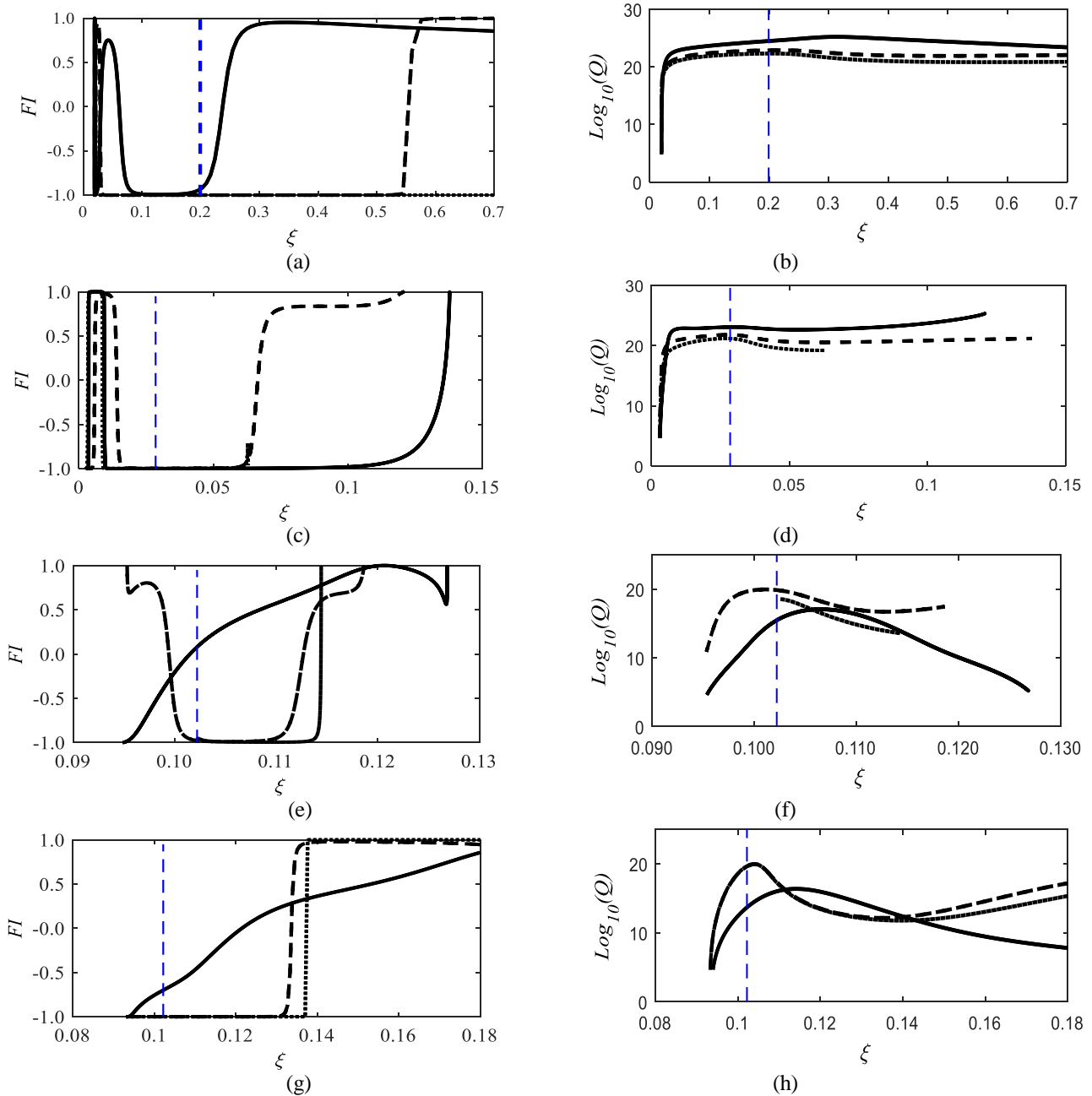


Fig. 5 Normalized flame index (a, c, e, g), logarithmic heat release rate ($\text{J/m}^3/\text{s}$) for reported conditions (b, d, f, h) at three different stream-wise directions for the cases 1 (a, b), 2 (c, d), 3 (e, f) and 4 (g, h). Solid line: $x=x_1$, dashed: x_2 , dotted: x_3 . Dashed blue vertical line (ξ_{st}) corresponds to the stoichiometric mixture fraction.

cosine of the angle between the fuel and oxidizer gradients, and thus, values of FI close to unity imply locally premixed, and negative FI values correspond to non-premixed.

Figure 5 shows the FI and the logarithmic heat release rate for half jet as a function of mixture fraction at different streamwise distances, x_1 , x_2 and x_3 . Here, x_1 corresponds to the most upstream location of a high heat release rate ($Q/Q_{max} = 0.8$), $x_2 = x_1 + 3.5$ mm, and $x_3 = x_2 + 7.0$ mm.

For the case 2, a conventional triple flame structure is formed. However, the relative location of diffusion flame branch and stoichiometric mixture fraction position is shifted for steam dilution case. For the case 3, the stoichiometric mixture fraction position is located almost at the boundary between the diffusion and lean premixed

flame branches. For case 4, this trend continues. Moreover, the lean premixed flame branch disappears in the case 4.

6. Summary

To understand the lifted flame structure, DNS have been carried out for laminar lifted flames for gas turbine relevant combustion phenomena. Although the present pressure is lower than nominal engine conditions due to the computational limitations, the other thermochemical conditions are carefully chosen to match the practical condition. For non-steam cases, it was observed that the flame base is relatively narrow in transverse direction compared to the steam dilution cases. The flame structure is analyzed by using normalized flame index to discuss the

flame structure near the flame base. For high pressure steam diluted cases, the lean premixed flame branch is disappeared yielding bibrachial structure in rich zone. The mechanism of this disappearance is to be investigated by looking into chemical kinetics in future.

7. References

- (1) Buckmaster, J. "Edge-flames". *Progress in Energy and Combustion Science*, Vol 28 (2002), pp. 435-475.
- (2) Buckmaster, J. and Weber, R., "Edge flame holding". *Proceedings of the Combustion Institute*, Vol.26 (1), (1996), pp.1143-1149.
- (3) Broadwell, J. E., Dahm, W. J. A. and Mungal, M. G., "Blowout of turbulent diffusion flames". *Proceedings of the Combustion Institute*, Vol.20 (1) (1985), pp.303-310.
- (4) Miake-lye, R. C. and Hammer, J. A., "Lifted turbulent jet flames: a stability criterion based on the jet large-scale structure". *Proceedings of the Combustion Institute*, Vol.22 (1) (1989) pp.817-824.
- (5) Krisman, A., Hawkes, E.R., Talei, M., Bhagatwala, A. and Chen, J.H., "Polybrachial structures in dimethyl ether edge-flames at negative temperature coefficient conditions". *Proceedings of the Combustion Institute*, Vol. 35 (2015), pp. 999-1006.
- (6) Tanahashi, M., Fujimura M. and Miyauchi T., "Coherent fine eddies in turbulent premixed flames". *Proceedings of the Combustion Institute*, Vol. 28 (2000), pp. 529-535.
- (7) Minamoto, Y., Fukushima N., Tanahashi, M., Miyauchi, T., Dunstan, T. D., and Swaminathan, N., "Effect of flow-geometry on turbulence-scalar interaction in premixed flames". *Physics of Fluids*, Vol.23 (2) (2011), pp.125107-1:18.
- (8) Aoki, K., Shimura, M., Ogawa, S., Fukushima, N., Naka, Y., Nada, Y., Tanahashi, M. and Miyauchi, T., "Short- and long-term dynamic modes of turbulent swirling premixed flame in a cuboid combustor". *Proceedings of the Combustion Institute*, Vol. 35 (2015), pp. 3209-3217.
- (9) Gou, X., Sun, W., Chen, Z., and Ju, Y., "A dynamic multi-timescale method for combustion modeling with detailed and reduced chemical kinetic mechanisms". *Combustion and Flame*, Vol. 157(6) (2010), pp. 1111-1121.
- (10) Sun, W., and Ju, Y., "A multi-timescale and correlated dynamic adaptive chemistry and transport (co-dact method for computationally efficient modeling of jet fuel combustion with detailed chemistry and transport." *Combustion and Flame*, Vol.184 (2010), pp. 297-311.
- (11) Sun, W., Gou, X., El-Asrag, H. A., Chen, Z., and Ju, Y., "Multi-timescale and correlated dynamic adaptive chemistry modeling of ignition and flame propagation using a real jet fuel surrogate model". *Combustion and Flame*, Vol.162 (4) (2015), pp. 1530-1539.
- (12) Poinso, T.J. and Lele, S.K., "Boundary conditions for direct simulations of compressible viscous flows". *Journal of Computational Physics*, Vol. 101 (1) (1992), pp.104-129.
- (13) Baum, M., Poinso, T.J. and Thévenin, D., "Accurate boundary conditions for multicomponent reactive flows". *Journal of Computational Physics*, Vol. 116 (1994), pp.247-261.
- (14) Burke, M.P., Chaos, M., Ju, Y., Dryer, F.L. and Klippenstein, S.J., "Comprehensive H₂/O₂ kinetic model for high-pressure combustion". *International Journal of Chemical Kinetics*, Vol. 44 (2011), pp. 444-474.
- (15) Li, J., Zhao, Z., Kazakov, A., and Dryer, F.L., "An updated comprehensive kinetic model of hydrogen combustion". *International Journal of Chemical Kinetics*, Vol. 36 (10) (2004), pp. 566-575.
- (16) Kee, R.J., Rupley, F.M, Meeks, E. and Miller, J.A., "Chemkin-II: A Fortran chemical kinetic package for the analysis of gas-phase chemical and plasma kinetics". *Technical Report SAND96-8216 Sandia National Laboratories* (1996).
- (17) Kee, R.J., Lewis, G.D., Warnatz, J., Coltrin, M.E. and Miller, J.A., "A Fortran computer code package for the evaluation of gas-phase multicomponent transport properties". *Technical Report SAND86-8246 Sandia National Laboratories* (1986).
- (18) Yoo, C.S, Richardson, E.S. and Sankaran, R. (2011): "A DNS study on the stabilization mechanism of a turbulent lifted ethylene jet flame in highly-heated coflow". *Proceedings of the Combustion Institute*, Vol. 33 (1), pp.1619-1627.
- (19) Ruetsch, G.R., Vervisch, L. and Liñán, A., (1995): "Effects of heat release on triple flames", *Physics of Fluids*, Vol. 7 (6), pp.1447-1454.
- (20) Bilger, R.W. (1988): "The structure of turbulent nonpremixed flames". *Proceedings of the Combustion Institute*, Vol. 22, pp.475-488.
- (21) Poling, B.E., Prausnitz, J.M. and O'Connell, J.P., "The Properties of Gases and Liquids". McGraw-Hill, New York (2001).
- (22) Kuznetsov, M., Redlinger, R., Breitung, W., Grune, J., Friedrich, A., and Ichikawa, N., "Laminar burning velocities of hydrogen-oxygen-steam mixtures at elevated temperatures and pressures". *Proceedings of the Combustion Institute*, Vol.33 (2011), pp. 895-903.
- (23) Yoo, C.S, Sankaran, R. and Chen, J.H., "Three dimensional direct numerical simulation of a turbulent lifted hydrogen jet flame in heated coflow: flame stabilization and structure". *Journal of Fluid Mechanics*, Vol. 640 (2009), pp.453-481.
- (24) Mastorakos, E., Baritaud, T. A. and Poinso, T. J., "Numerical simulations of autoignition in turbulent mixing flows". *Combustion and Flame*, Vol. 109 (1997), pp.198-223.
- (25) Yamshita, H., Shimada, M. and Takeno, T., "A numerical study on flame stability at the transition point of jet diffusion flames". *Proceedings of the Combustion Institute*, Vol.26 (1) (1996), pp.27-34.
- (26) Mizobuchi, Y., Tachibana, S., Shinio, J., Ogawa, S. and Takeno, T., "A numerical analysis of the structure of a turbulent hydrogen jet lifted flame". *Proceedings of the Combustion Institute*, Vol.29 (2002), pp. 2009-2015.