

Numerical study on the behavior of non-premixed flames in twin-jet counterflow with one-step reaction model

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Abstract: The structure of a non-premixed flame in a twin-jet counterflow was simulated using reduced and detailed mechanisms for methane fuel diluted with nitrogen. A non-premixed flame with an advancing edge was stabilized with a trail flame, similarly to a conventional counterflow flame. At large strains, the trailing flames were extinguished, such that a petal-shaped flame with a retreating edge existed. Various types of methane non-premixed flames (conventional counterflow flame, fuel-sharing and oxidizer-sharing crossed twin-jet counterflow flames, and petal-shaped flame) were simulated in the twin-jet counterflow configuration depending on the combination and dilution of the initial fuel and oxidizer supplied to each nozzle. The cross-condition in the twin-jet counterflow flames coincided with the transition from fuel-to oxidizer-sharing flames. In particular, the extinction characteristics of methane non-premixed flames were investigated in crossed twin-jet counterflow configuration. In addition, petal-shaped flames existed only in the region favoring the formation of oxidizer-sharing flames.

Keywords: Twin-jet counterflow, Facing curved flames, Cross-condition, Extinction, Petal-shaped flame

1. Introduction

Turbulent flames, which are involved in most combustion applications of practical interest, are assumed to be composed of an ensemble of laminar flamellets with different intensities and extents [1]. The structure and extinction of laminar flames in a counterflow configuration have been extensively investigated using the laminar flamellet model for non-premixed turbulent flames because of its convenience in experimental, numerical, and theoretical approaches [2]. Turbulent non-premixed flames can be highly curved; therefore, an appreciable interaction with a neighboring flame surface is expected [3]-[5]. In addition, non-premixed flames can experience negative strain in turbulent flows [6].

However, the realization of the effects of curvature, negative strain, and interaction of non-premixed flames is limited in a conventional counterflow configuration. Therefore, a two-dimensional “twin-jet counterflow” burner, in which two double-slit nozzles formed a counterflow, was proposed in [7].

In this study, a numerical simulation of twin-jet counterflow was conducted to investigate the mechanisms of the extinction and interaction of non-premixed methane flames and the formation of petal-shaped flames.

2. Numerical simulation

To simulate the extinction and interaction of twin-jet counterflow flames, time-dependent governing equations in rectangular coordinates (x, y) were solved for the momentum, species, and energy equations. A one-step overall reaction mechanism, $\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$, was adopted to account for the enthalpies of formation. Compared to detailed chemistry modeling, this one-step mechanism has limitations in explaining the detailed flame structure because it cannot account for the interactions between the intermediate species in premixed and diffusion edge-flames. However, the hydrodynamic and thermal fields and qualitative nature of the flame response can be described reasonably using the mechanism. The activation energy of methane/air, E_a , was chosen as 48.0 kcal/mole [8]. The pre-exponential factor A was selected as 8.3×10^{16} after a comparison with the experimental extinction condition of a conventional counterflow flame. The thermodynamic and transport properties were calculated using CHEMKIN-III and TRANSPORT packages [9], respectively.

As shown in **Figure 1**, the computational dimensions were 2 cm \times 1 cm, and the numbers of meshes were 256 and 128 in the x and y directions, respectively. A uniform flow was assumed at

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the inlet. At the outlet, all scalar and velocity vectors were evaluated based on convective boundary conditions. A test with a double-grid system (512×256) showed no difference in the flame structure. The slip-wall boundary condition was used to minimize the effect of the boundary conditions at the sidewalls. Finally, the buoyancy effect was not included.

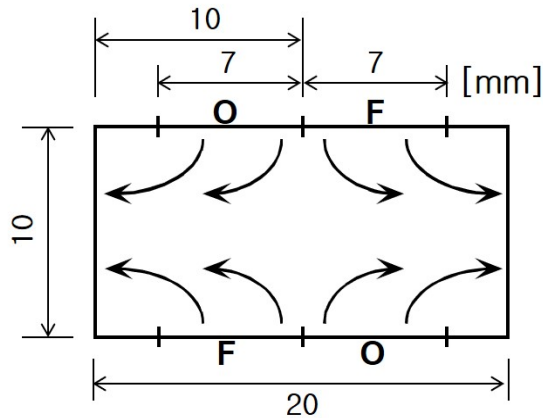


Figure 1: Calculation domain of twin-jet counterflow config

3. Results and discussion

3.1 Various twin-jet counterflow flames

Four different types of twin-jet counterflow flames were observed, depending on the combination of the initial fuel and oxidizer supplied to each nozzle, as shown in **Figure 2**. The numerical condition $X_{O,0} = 0.26$ was maintained, where X is the mole fraction and the subscripts F, O, and 0 denote fuel, oxidizer, and the nozzle exit, respectively, and the exit velocity was fixed at $V_{in} = 10$ cm/s. A conventional counterflow non-premixed flame was observed, as shown in **Figure 2(a)**, when the fuel and oxidizer were supplied through the lower and upper nozzles, respectively. By supplying fuel and oxidizer in the cross-stream arrangement, two highly curved non-premixed flames were observed, as shown in **Figures 2(b)** and **(c)**. This study mainly focused on these flames to investigate the extinction of non-premixed methane flames. These flames consisted of two sections: a horizontal wing section resembling a conventional counterflow flame and a vertical section resembling a vertical flame in the parallel stream, such as that observed in the mixing layer. Consequently, the crossed twin-jet flame exhibited the characteristics of a non-premixed flame and a partially premixed flame. The crossed twin-jet flame near the extinction limit condition changed into a petal-shaped flame when both wings were extinguished, as shown in **Figure 2(d)**. When a petal-shaped flames form, the extinction boundary of crossed twin-jet

counterflow flames can be extended beyond that of conventional counterflow non-premixed flames.

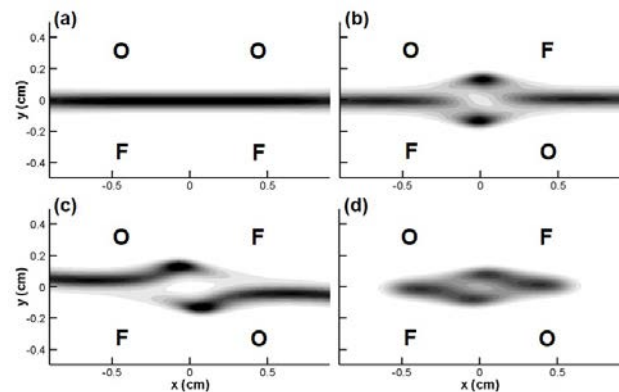


Figure 2: Heat release contours of various non-premixed flames for $X_{O,0} = 0.26$ and $V_0 = 10$ cm/s with the combination and dilution of fuel and oxidizer supplied to each slit

3.2 Fuel and oxidizer sharing flame

The characteristics of the flames in the crossed twin-jet counterflow can vary depending on the concentration of the fuel and oxidizer supplied to each slit. The flame behavior under various concentrations of the reactants was observed. To facilitate the comparison among different flames, the fuel and oxidizer mole fractions ($X_{F,0}$, $X_{O,0}$) at the inlet were varied such that the adiabatic flame temperature of the counterflow flame was kept constant. The adiabatic flame temperature, T_{ad} , was obtained from the free-stream stoichiometric mixture of the fuel and oxidizer.

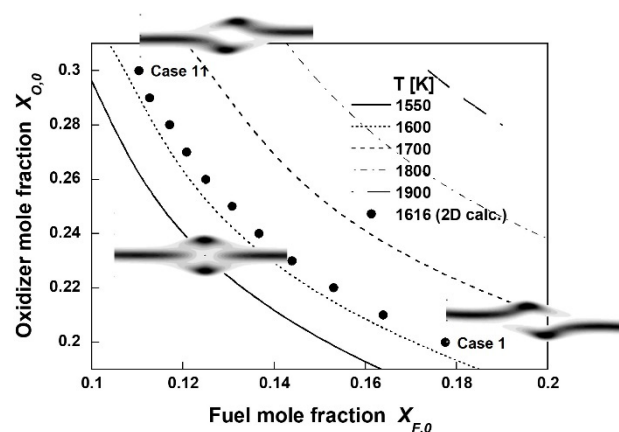


Figure 3: Iso-condition map of twin-jet counterflow flames at $V_0 = 10$ cm/s under constant adiabatic flame temperature

Several iso-adiabatic temperature lines are shown in **Figure 3**, and the selected conditions for the simulation, which are very close to the extinction limit of the conventional counterflow

flame, are marked for $T_{ad} = 1616$ K in the $X_{F,0}-X_{O,0}$ plot (case 1–11). According to the overall behavior, flames could be classified as fuel-sharing and oxidizer-sharing flames. When $X_{F,0}$ was large, the flames enclosed the oxidizer streams, and the two flames shared fuel between the two curved flame sections. Therefore, the flame was called a fuel-sharing flame in the cross stream. Under a large $X_{O,0}$, the flames enclosed the fuel streams; hence, the two curved flames were oxidizer-sharing.

3.3 Extinction characteristics

The extinction of the crossed twin-jet counterflow flames was a unique phenomenon. The behavior of the twin-jet counterflow flames at $V_{in} = 10$ cm/s in terms of $X_{F,0}$ and $X_{O,0}$ is depicted in **Figure 4**. The experimental extinction limits of non-premixed methane flames in the twin-jet counterflow configuration and that under the cross-flame condition were plotted. The extinction limit of the horizontal wing section is marked as a curved thick solid black line-dashed line, which corresponds to the boundary between extinction limits of the flames in the cross-stream configuration with complete wings and the flame with wings extinguished to form a petal-shaped flame. The complete extinction limit is marked by a thick, curved solid line. Here, the cross-flame condition, marked as a straight dotted line, denotes the boundary between the oxidizer and fuel-sharing flames.

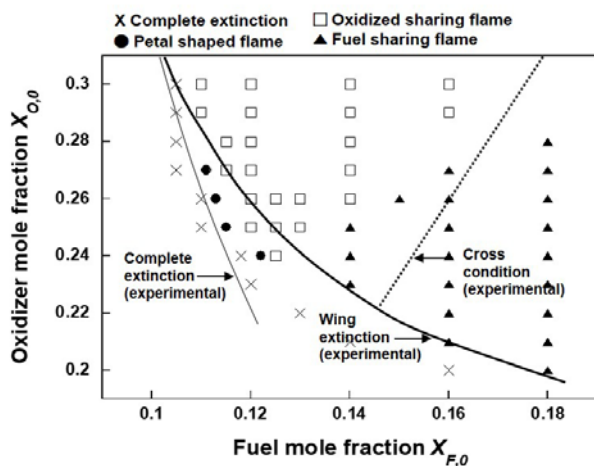


Figure 4: Extinction diagram for twin-jet counterflow configuration at $V_0 = 10$ cm/s

The open squares denote the measurements obtained for the oxidizer-sharing flames, solid triangle; for the fuel-sharing flames, solid diamond for petal-shaped flames, and cross; for petal-shaped flames. The experimental extinction limits of the twin-jet counterflow flame agreed reasonably well with the

numerical results. It should be noted that petal-shaped flames existed only in the region favorable to oxidizer-sharing flames.

The controlling parameters in determining the extinction conditions in the twin-jet counterflow were the fuel and oxidizer concentrations and jet velocity (V_0). In a previous experiment [7], the fuel concentration was varied using a fixed oxidizer concentration and jet velocity.

The present numerical results showed that the $X_{F,0}$ at which wing extinction occurred reduced as $X_{O,0}$ increased. In addition, petal-shaped flames were not observed at $X_{O,0} < 0.22$ (only in the fuel-sharing region). In this region, the distance between the facing curved flames was relatively higher than that between oxidizer sharing flames. Compared with the extinction limit of the conventional counterflow flame (nearly coinciding with the wing extinction in **Figure 4**), the extinction limits of the crossed twin-jet counterflow flame were extended when the petal-shaped flames were formed.

The mechanism of the extension of the extinction limits of crossed twin-jet counterflow flames is analyzed as follows. To identify the interaction between the flames in the cross-flow configuration, the maximum temperature of each flame was monitored. The temperature of the conventional counterflow flame were also calculated using the proposed two-dimensional simulation code.

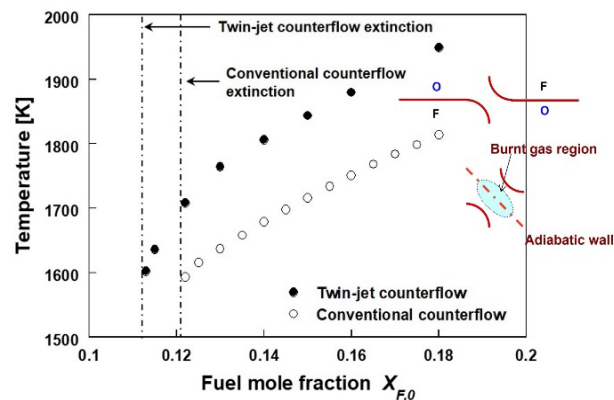


Figure 5: Maximum temperatures of conventional and crossed twin-jet counterflow flames under various fuel mole fraction $X_{F,0}$ for $X_{O,0} = 0.26$ and $V_0 = 10$ cm/s

The maximum temperature profiles of the conventional and twin-jet counterflow flames at $X_{O,0} = 0.26$ and $V_{in} = 10$ cm/s are shown in **Figure 5**, corresponding to the oxidizer-sharing flames. As the fuel mole fraction decreased, the maximum temperature of the conventional counterflow flame decreased and the flame was finally extinguished at $X_{F,0} = 0.122$. The maximum

temperature of the twin-jet counterflow flame also exhibited a similar behavior; however, the flame extinction occurred at a lower value of $X_{F,0} = 0.11$. Note that in the range $0.11 < X_{F,0} < 0.122$, the wing sections were extinguished such that petal-shaped flames were exhibited. This indicated that the extinction limit of crossed twin-jet counterflow flames was appreciably extended by the formation of petal-shaped flames.

The maximum temperature of the crossed twin-jet flame was approximately 100 K higher than that of the conventional counterflow flame in the oxidizer sharing condition ($X_{F,0} < 0.140$). The maximum temperature in the conventional counterflow flame occurred in the wing section. The maximum temperature of the crossed twin-jet flame was located either at the leading-edge flame or at the stagnation point, depending on the combination of the fuel and oxidizer mole fractions.

3.4 Extinction characteristics

To demonstrate the effect of an adiabatic wall between the interacting flames clearly, the temperature profiles along the shortest distance between the maximum heat release positions of two facing curved flames in the fuel sharing, oxidizer sharing, and petal-shaped flame regimes are shown in **Figure 6**.

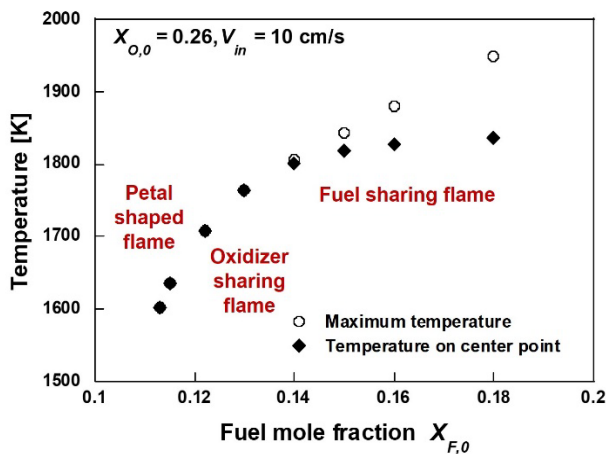


Figure 6: Maximum temperature and temperature at the center point with various fuel mole fraction $X_{F,0}$ for $X_{O,0} = 0.26$ and $V_0 = 10$ cm/s

The results showed that the maximum value of temperature was obtained at the center for the oxidizer-sharing and petal-shaped flames. The temperature at the center of the fuel-sharing flames showed a local minimum. For the oxidizer-sharing flames, the temperature at the center showed the maximum value. Therefore, in fuel sharing flames, heat loss occurred toward the

center region, whereas no heat flux was observed toward the center in the oxidizer sharing flames, indicating the adiabatic nature of the two interaction flames.

The overall trends of the adiabatic wall effect in the crossed twin-jet counterflow and petal-shaped flames can be inferred from the two-dimensional temperature contours shown in **Figure 7**, which shows the maximum temperature in the center region. It should also be noted that the temperature in petal-shaped flames exhibited a decreasing trend along the horizontal wings.

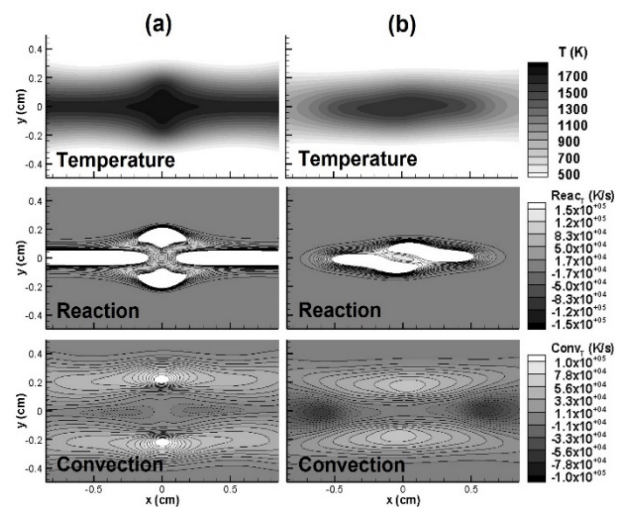


Figure 7: The contours of temperature, reaction and convection for (a) crossed twin-jet counterflow flame and (b) petal shaped flame

The reaction rate of the petal-shaped flame similarly decreased gradually along the wings, and finally, extinction occurred at the end of the horizontal flame wings. This type of flame boundary between the reacting and quenched regions can be regarded as the retreating edge flame because the direction of the edge flame propagation toward the unburned mixture is same as to that of the local flow velocity, and the flame edge is maintained as a standing flame. Therefore, investigating petal-shaped flames could be worthwhile because one can observe the retreating edge flame as a standing wave [10].

However, while measuring the retreating edge speed, directly defining the feasible position of the edge flame is slightly impractical because of the gradually decreasing nature of the temperature and reaction rate around the edge region. To arrive at a reasonable definition of the edge position, each term in the energy equation in the numerical simulation was monitored using the steady formulation given in **Equation (1)**, which is composed of the convection, diffusion, and reaction terms. In the

steady case, the convection heat flux is a combination of diffusion and reaction heat fluxes.

$$\vec{u} \cdot \nabla T = \frac{\nabla \cdot (\lambda \nabla T)}{\rho c_p} + \frac{\omega_r}{\rho c_p}, \quad (1)$$

where, T is the temperature, \vec{u} is the flow velocity, ρ is the density, c_p is the specific heat, and ω_r is the heat release rate by the reaction. The convection heat flux contours of the crossed twin-jet counterflow and petal-shaped flames are shown in **Figure 7** for $V_0 = 10$ cm/s and $X_{O,0} = 0.26$. The solid and dotted contours denote the heat gain and heat loss in the control volume, respectively. The convection field of the crossed twin-jet counterflow flame (**Figure 7a**) demonstrated that the upper and lower regions of the horizontal stagnation line were heated via heat diffusion from the reacting zone; however, the heat near the central region was diffused inversely. The petal-shaped flame (**Figure 7b**) exhibited a similar trend as that of crossed twin-jet counterflow flame, except that the two largest heat loss regions occurred near the retreating edge flame, where cold unburned mixtures flew. In addition, the heat loss regions have a unique minimum point in the valley with the physical meaning of the maximum heat-loss point. Based on these characteristics, the retreating edge point can be regarded as the minimum point of the convection heat flux.

4. Conclusion

Various types of non-premixed flames were observed in the twin-jet counterflow burner, depending on the combination of the fuel and oxidizer supply through each slit. In particular, the extinction characteristics of non-premixed methane flames were investigated in cross-stream twin-jet flames. Owing to the formation of petal-shaped flames, the extinction boundary became wider than that of conventional counterflow non-premixed methane flames through the interaction of the curved section of the flames. The cross-flame condition was investigated in the cross-stream counterflow configuration, and petal-shaped flames were observed in the oxidizer-sharing flame region. Four different types of methane non-premixed flames (conventional counterflow flame, fuel-sharing and oxidizer-sharing crossed twin-jet counterflow flames, and petal-shaped flame) were investigated in the twin-jet counterflow configuration depending on the combination of the initial fuel and oxidizer

supplied to each nozzle. In particular, the extinction characteristics of methane non-premixed flames were investigated in crossed twin-jet counterflow configuration. The extinction boundary of crossed twin-jet counterflow flames can be extended more than that of conventional counterflow non-premixed flames. The experimental extinction boundary of the twin-jet counterflow flames at a fixed stretch rate agreed reasonably well with the numerical results. In addition, petal-shaped flames existed only in the region favoring the formation of oxidizer-sharing flames. The extinction limits of interacting non-premixed flames were extended by the formation of petal-shaped flames. An analysis of the temperature profiles along the shortest distance between the maximum heat release positions of the two facing curved flames revealed that an adiabatic wall was formed on the crossed twin-jet counterflow oxidizer-sharing flames. To arrive at a reasonable definition of the edge position, each term of the energy equation in the numerical simulation was monitored using the steady formulation. From this analysis, it can be concluded that the retreating edge point can be regarded as the minimum point of the convection heat flux.

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Author Contributions

Resources, K. W. Chun; Writing-Original Draft Preparation, K. W. Chun; Writing-Review & Editing, K. W. Chun.

References

- [1] N. Peters, *Turbulent Combustion*, Cambridge University Press, Cambridge, 2000.
- [2] F. A. Williams, "Progress in knowledge of flamelet structure and extinction," *Progress in Energy and Combustion Science*, vol. 26, no. 4-6, pp. 657-682, 2000.
- [3] S. H. Sohrab and B. H. Chao, "Influences of upstream versus downstream heat loss/gain on stability of premixed flames," *Combustion Science and Technology*, vol. 38, no. 5-6, pp. 245-265, 1984.
- [4] S. H. Sohrab, Z. Y. Ye, and C. K. Law, "An experimental investigation on flame interaction and the existence of negative flame speeds," *Symposium (International) on Combustion*, vol. 20, no. 1, pp. 1957-1965, 1985.

- [5] S. H. Sohrab, Z. Y. Ye, and C. K. Law, "Theory of interactive combustion of counterflow premixed flames," *Combustion Science and Technology*, vol. 45, no. 1-2, pp. 27-45, 1986.
- [6] N. Peters, "Laminar flamelet concepts in turbulent combustion," *Symposium (International) on Combustion*, vol. 21, no. 1, pp. 1231-1250, 1988.
- [7] S. Y. Yang, B. K. Lee, and S. H. Chung, "Observation of various non-premixed flames in twin-jet counterflow," *Combustion and Flame*, vol. 136, no. 1-2, pp. 246-248, 2004.
- [8] R. J. Kee, F. M. Rupley, E. Meeks, and J. A. Miller, *CHEMKIN-III: A Fortran Chemical Kinetics Package for the Analysis of Gas-phase Chemical and Plasma Kinetics*, Report No. SAND96-8216, U.S. Department of Energy Office of Scientific and Technical Information, USA, 1996.
- [9] A. Liñán, "The asymptotic structure of counterflow diffusion flames for large activation energies," *Acta Astronautica*, vol. 1, no. 7-8, pp. 1007-1039, 1974.
- [10] J. Buckmaster, "Edge-Flames," *Progress in Energy and Combustion Science*, vol. 28, no. 5, pp. 435-475, 2002.