Numerical Study on Ultra-Lean Premixed Flame in Swirl Flow with Recirculating of Burned Gas including Active Radicals

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1 Introduction

Lean combustion has some advantages such as high efficiency of fuel utilization and reduction of NOx emission [1]. If ultra-lean combustion whose equivalence ratio is out of the lean flammability limit is realized, we can increase the fuel utilization efficiency further. However, it is usually impossible to realize ultra-lean combustion without preheating.

Our research group numerically studied on the vortex bursting phenomenon and found that the flame at the propagating front is not extinguished despite its high propagation speed and the large flame stretch rate at the tip [2]. This result led us to an idea of ultra-lean combustion by utilizing swirl flow without preheating. Recently, we have numerically studied on a methane-air co-rotating counterflow twin premixed flame (RCTF) shown in Fig. 1 with a detailed chemical kinetics, and revealed that an ultra-lean flame of equivalence ratio $\phi = 0.32$ can be formed [3]. In the case of a RCTF, when the rotating number exceeds a critical value a backflow region is formed due to the centrifugal force. And it was found that in the ultra-lean condition a stagnation point x_{stag} is located within the flame zone. Figure 2 compares the ultra-lean flame structures of a planar one-dimensional premixed flame and a RCTF, whose equivalence ratios are both 0.35. It must be noted that even under such a lean equivalence ratio the planar one-dimensional premixed flame can be computationally obtained though it definitely cannot be realized experimentally. In the case of RCTF, the reactants are transported by diffusion against convection over the stagnation point. This implies that the local flame speed can be negative in a stable premixed combustion.

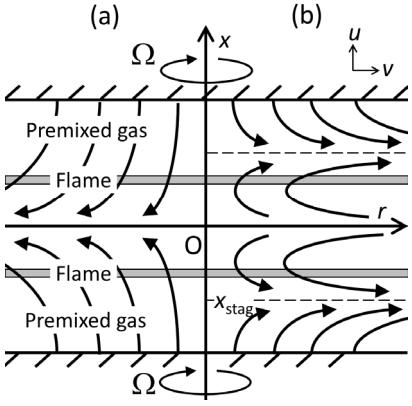

Figure 1. Schematic of co-rotating counterflow twin flame. The cases of (a) small rotating number and (b) large rotating number.

It is well known that under lean conditions near the flammability limit radiative heat loss largely affects the structure and the stability of premixed flames [4]. Accordingly, we found that the leanest extinction limit of RCTFs are shifted from $\phi =$ 0.32 to 0.42 by adopting an optically thin radiative heat loss model for four major species. In this result, however, the radiative heat loss may have been overestimated since the model does not include the effect of radiative reabsorption at all. So it must be essential to validate the obtained computational results by experiments, but it is practically impossible to perform an experiment of high-rotating-number co-rotating counterflow twin

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flame of infinitely large radius that have been simulated based on a similarity solution. Therefore, for validating the abovementioned ultra-lean combustion phenomenon experimentally, we have to adopt a flame of more realistic configuration as a target.

As a flame of such configurations, recently we designed an axisymmetric 2-D swirl flame model shown in Fig.3, which will be able to be realized experimentally. In this flame the backflow by recirculation flow of burned gas occurs similarly to the RCTF. In this paper, we report the numerical results as the first step of the study on the flame. In particular, we focus on the structure of an ultra-lean flame and the concentrations of species including active radicals in the burned gas.

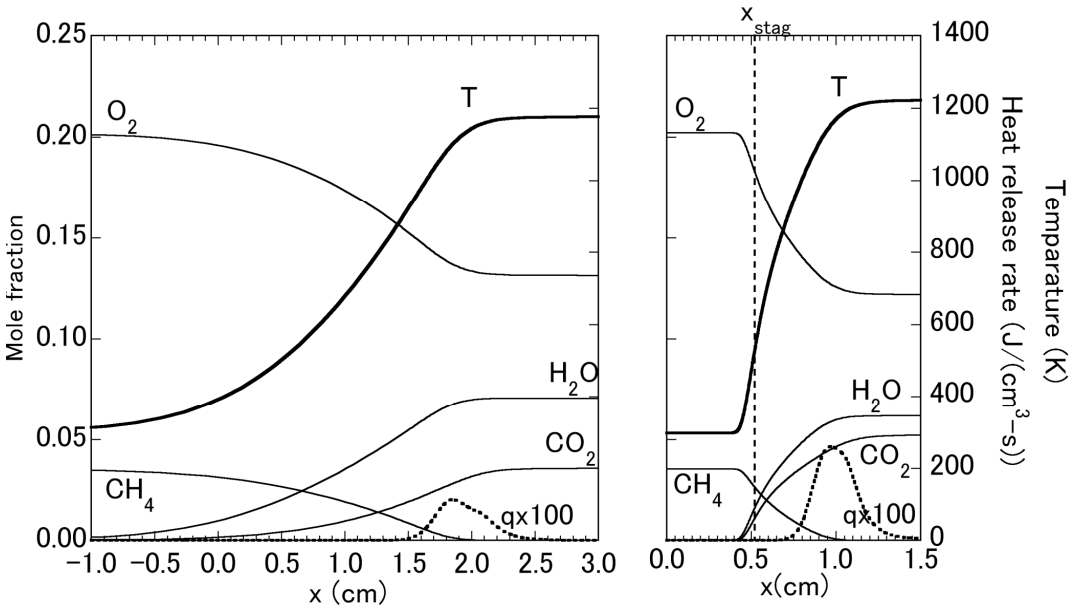

Fig. 2. Ultra-lean flame structure of ϕ = 0.35. Left: an ordinary one-dimensional premixed flame. Right: a rotating counter-flow twin flame (u_R = 200 cm/s, Ω = 150 rps)

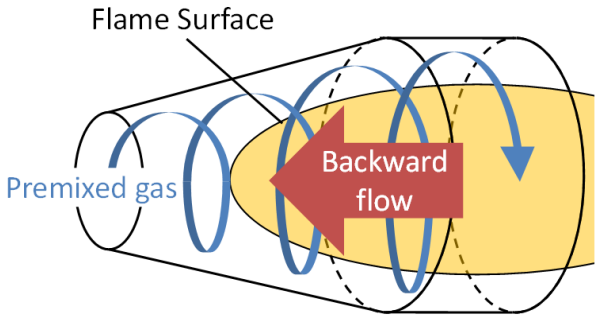

Fig. 3. Schematic of an axisymmetric swirl burner in which the swirling flow field with a recirculation zone can be treated two-dimensionally.

2 Numerical Method

We assumed an axisymmetric two-dimensional flow. Governing equations are the equation of continuity, Naviar-Stokes equation, and conservation equations for energy and concentrations of all species. These equations were discretized and solved computationally with the equation of state of ideal gas. Figure 4 shows a calculation domain and boundary conditions. At the inlet x = 2.0 cm, we gave the upstream boundary conditions of unburned gas: temperature T_0 = 300 K, the species mass fractions $Y_{k,0}$, the axial

velocity U, and the circumferential velocity $w = W(r)$. For $W(r)$, we assumed Burgers' vortex and gave the distribution as below:

$$W(r) = \frac{\Gamma}{2\pi r}\left[1 - \exp\left\{-\frac{r^2}{(\sigma_0/2)}\right\}\right]$$

Γ, σ_0 are the velocity circulation and the initial diameter of the vortex core. In this study we assumed $\sigma_0 = 2.0$ cm. The numerical code is based on SIMPLE scheme [5] and CHEMKIN subroutine libraries [6-8] for evaluating chemical reaction rates, thermochemical properties and transport properties. The adapted chemical kinetics scheme is somewhat simplified C1 chemistry obtained by deleting all NOx-related reactions from GRI-mech3.0 [9]. The resultant scheme involves 23 species and 119 elementary reactions.

First, to simplify the physics, we simulated the flame without radiative heat loss. Then the "optically thin model" proposed by Barlow et al [9] was included for evaluating the effect of radiation. The following radiative heat loss term was added to the energy conservation equation.

$$q_r = -4\sigma\left(T^4 - T_0^4\right)\sum_{k=1}^{K} p_k a_{p,k}$$

where σ, T, T_0 are the Stefan-Boltsmann's constant, the local flame temperature, the background temperature, and p_k, $a_{p,k}$ are the partial pressure of gas, the Planck mean absorption coefficient for k^{th} species, respectively. The Planck mean absorption coefficients were calculated only for CO_2, H_2O, CH_4 and CO. Reabsorption of radiation is not considered, so all the radiated heat is simply regarded as heat loss.

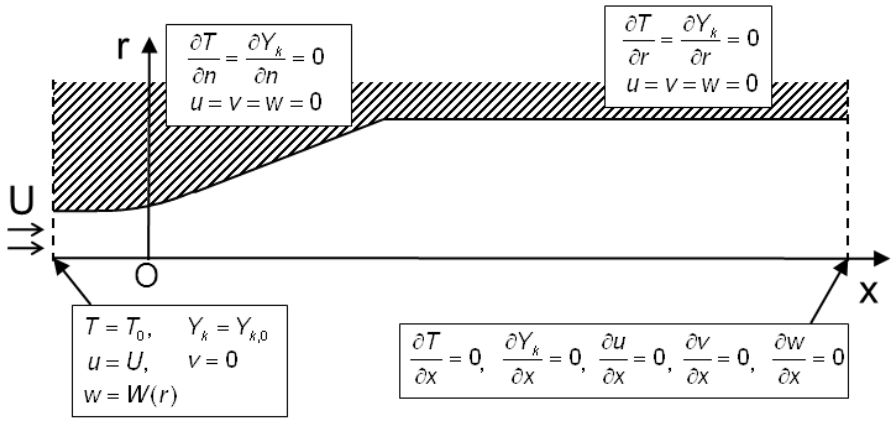

Fig. 4. Calculation domain and boundary conditions.

3 Results and Discussions

3.1 Ultra-Lean 2D Swirl Flame Structure

We obtained an ultra-lean flame of $\phi = 0.35$. Figures 5 and 6 respectively show the distributions of temperature and velocity calculated without radiative heat loss. It is seen in Fig.5 that the flow is complicated and a number of vortices are formed. Near the flame tip, there exists a stagnation point between the unburned gas and the backflow of the burned gas, and a recirculation zone is formed along the shoulder of the flame surface following the flame tip. The flame surface remains stable, steady and smooth near the flame tip despite the large fluctuation of the downstream flow. This fluctuation seems to occer because the cold unburned gas breaks into the hot burned gas which recirculates to the flame zone and weakens the flame. In this region, the winkled flame surface causes the complicated, unsteady and unstable downstream flow. Reactants from the inlet impinge the high-temperature burned gas containing active radicals, which enhances and stabilizes the ultra-lean flame around the tip. Figure

7 shows the flame structure on the center axis of the flame shown in Figs. 5 and 6. The stagnation point x_{stag} where the axial velocity u = 0.0 cm/s is indicated by a broken line. It is seen that the stagnation point is located within the preheat zone and the reaction zone is located in the backflow region beyond x_{stag}. The same special relationship between the stagnation point and the reaction zone is basically the same as that of the RCTF shown in Fig. 2.

We next performed the calculation for the same conditions as the one in Figs. 5 and 6 with radiative heat loss. Figure 7 compares the flame structure on the axis between with and without radiative heat loss. The left part of the figure shows the case with radiation, while the right part shows the case

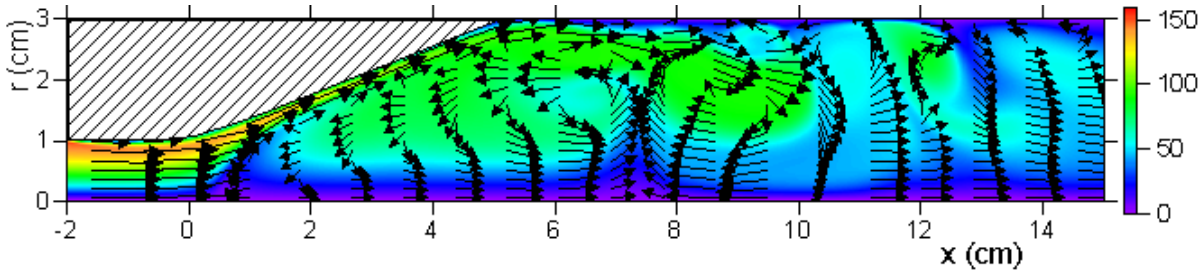

Fig. 5. Velocity distribution (without radiation). Unit is cm/s. Color graduation shows the circumferential velocity. ϕ = 0.35, U = 150 cm/s, W_{max} = 150 cm/s.

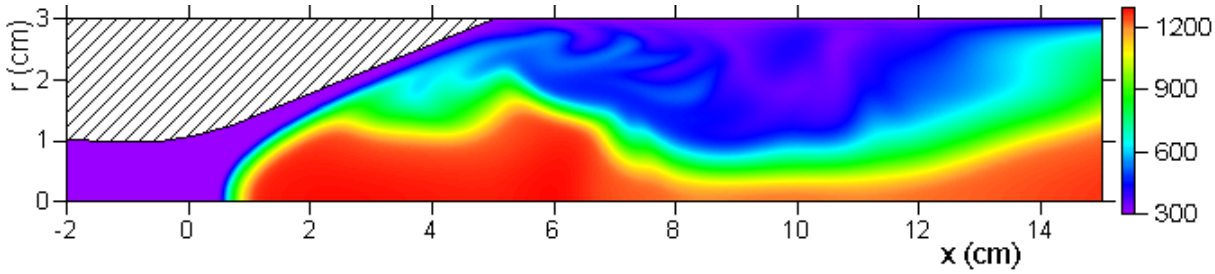

Fig. 6. Temperature distribution (without radiation). Unit is K. ϕ = 0.35, U = 150 cm/s, W_{max} = 150 cm/s.

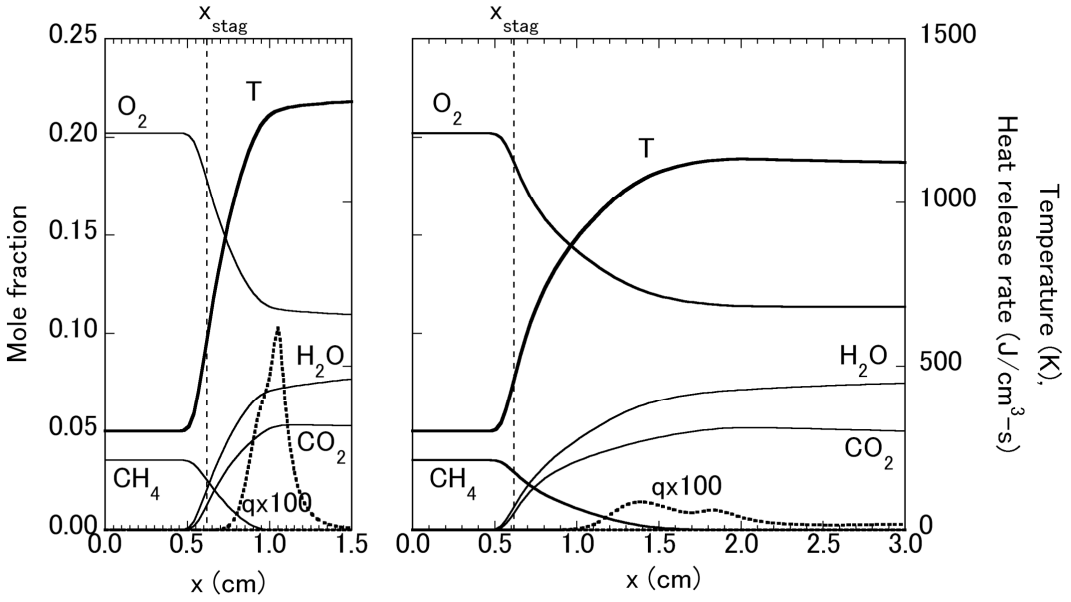

Fig. 7. Two-dimensional swirl flame structure of ϕ = 0.35. Left: without radiation heat loss. Right: with radiation heat loss. For each result, calculation conditions are U = 150 cm/s, W_{max} = 150 cm/s.

without it. Although the flame temperature T and the heat release rate q are largely decreased by the radiative heat loss, the fundamental structure of the flame is almost unchanged and all the profiles do not change largely with time. That is, a stable ultra-lean flame of $\phi = 0.35$ can be formed numerically even with radiative heat loss that might be overestimated, which suggests that the flame can probably be realized experimentally.

3.2 Burned Gas Species Including Active Radicals

Next we examined the composition of the backflowing burned gas, since it is thought to affect the reaction zone strongly via the direct convective transport from behind. Figure 8 compares the concentrations of the three major species in the burned gas of the ultra-lean premixed combustion of $\phi = 0.35$, among the equilibrium state, the RCTF, and the two-dimensional swirl flame. We selected the results without radiative heat loss, since the equilibrium state cannot be realized with the optically thin radiation model. The burned gas at $x = 0$ on the axis was chosen for the RCTF, while that at $x = 3.0$ cm on the axis was chosen for the two-dimensional swirling flame. It is seen that the composition is quite different among the three types of combustion even though the unburned gas is completely the same. It is interesting to note that the composition of the two-dimensional swirl flow corresponds to that of the equilibrium in a richer condition than $\phi = 0.35$.

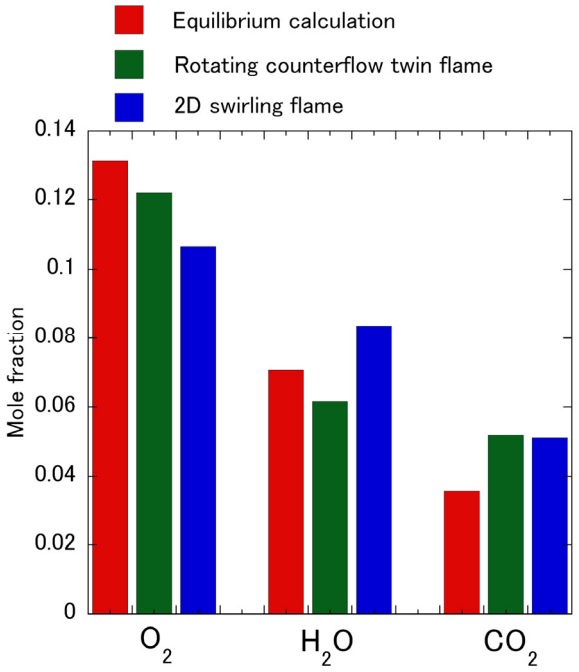

Fig. 8. Mole fractions of O_2, H_2O and CO_2 in the burned gas of $\phi = 0.35$.

Table 1 shows the mole fractions of the representative active radicals, O, OH and H. It must be emphasized that the concentrations of all the three chain-carrier radicals both in the cases of the RCTF and the two-dimensional swirl flame are much larger than those of the equilibrium state. We think that the larger radical concentrations in the burned gas of the two flames make it possible to realize the stable flames under the ultra-lean conditions.

Table 1: Mole fractions of active radicals O, H, OH in ultra-lean burned gas of $\phi = 0.35$.

	Equilibrium calculation	Rotating counterflow twin flame (u_R = 400 cm/s, W = 150 rps)	2D swirl burner (U = 150 cm/s, W_{max} = 150 cm/s)
O	5.42×10^{-9}	1.26×10^{-5}	5.02×10^{-7}
H	4.83×10^{-12}	6.04×10^{-7}	3.93×10^{-9}
OH	1.61×10^{-6}	6.94×10^{-5}	1.57×10^{-5}

4 Concluding Remarks

We numerically performed the ultra-lean premixed flame of $\phi = 0.35$ in a swirl flow which can be treated two-dimensionally and compared to experiment. Its flame structure is similar to a rotating counterflow twin flame, i.e., an additional stagnation point is formed within the flame zone and fresh species are transported from upstream to the flame surface not by convection but by diffusion over the stagnation point. These structures are quite different from an ordinary premixed flame. Moreover, not

only the flame structure but also the burned gas composition are different. The burned gas includes much more active radicals such as O, H, and OH than the equilibrium composition (1D premixed flame). From these, ultra-lean flame can be formed. It was revealed that not only in the case of a rotating counterflow twin flame, an ultra-lean flame can be realized where the premixed gas and the burned gas are countered

References

[1] Dunn-Rankin D. (2008). Lean Combustion. Elsevier (ISBN 0-12-370619-X).

[2] Nishioka M, Hokazono T. (2005). Effect of Local Flame Stretch at the Tip of the Flame Propagating in a Vortex. 20th Int. Colloquium on the Dynamics of Explosions and Reactive Systems, Canada.

[3] Nishioka M, et al. Ultra-Lean Combution Mechanism by Backflow of Burned Gas in Swirling Counterflow Premixed Flame. Combustion and Flame (in printing, doi: 10.1016/j.combustflame.2011.04.002).

[4] Ju Y, Maruta K, Niioka T. (2001) Combustion Limits. Appl. Mech. Rev. 54: 257.

[5] Patankar SV. (1980). Numerical Heat Transfer and Fluid Flow. Hemisphere Publishing Corporation (ISBN 0-89116-522-3).

[6] Kee RJ et al. (1985). Sandia Report, SAND 85-8240.

[7] Kee RJ et al. (1986). Sandia Report, SAND 86-8246.

[8] Kee RJ, Rupley FM, Miller JA. (1989). Sandia Report, SAND 89-8009.

[9] Smith GP et al. http://www.me.berkeley.edu/gri-mech/

[10] Barlow RS et al. (2001). Scalar Profiles and NO Formation in Laminar Opposed-Flow Partially Premixed Methane/Air Flame. Combustion and Flame. 127: 2102.