Radiative Extinction Characteristics of Low-Lewis-Number Counterflow Premixed Flame in Microgravity and Its Correlation with Flame Ball

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1 Introduction

For low-Lewis-number mixture, transition from planar flame to cellular flames occurs due to diffusive-thermal instability [1]. Experiments using counterflow slot-jet H₂/air premixed flames have shown a transition from two nearly planar flames to stationary flame tubes with a decrease of equivalence ratio [2]. The transition of flames is due to thermal-diffusive instability.

Our previous experiments using CH₄/O₂/CO₂ versus O₂/CO₂ counterflow diffusion flames at pressure above 0.5 MPa have shown that stretch rate at extinction monotonically decreases with a decrease of fuel mole fraction and reaches to the stretch rate lower than 50 s⁻¹ [3]. Then, a ‘cap-like’ flame, which appears to have some similarities with flame ball, has been observed in such condition, probably because of diffusive-thermal instability [3]. The observed diffusive-thermal instability has been due to the sufficiently lower Lewis number of fuel-lean CH₄/O₂/CO₂ mixture than unity.

However, reliable low-stretch-rate experiments is limited to, say, around 30 s⁻¹ [3] due to the effect of gravity. By gravity-free, long duration experiments in the space, the transition from counterflow premixed flames to a flame ball would be obtained using fuel-lean and low-Lewis-number mixture in extremely low stretch rate. Such experiments enable us to construct unified flammability theory including both deflagration wave and flame ball. The objectives of the present study are examinations of the possibility of transition from near-limit counterflow premixed flames to a flame ball. Numerical simulation with detailed chemistry was conducted as preliminary computation for future space experiment. Furthermore, results of microgravity experiment using airplane, which were obtained very recently, were presented together with the computational results.

2 Computation method

Computations for counterflow premixed flames were conducted by PREMIX-based 1-D flame code [4]. Computations for flame ball were conducted by PREMIX-based 1-D spherical flame code. The governing equations of 1-D spherical flame code were shown in the equation (2.1) and (2.2).
Species conservation equation:

\[ 0 = -\frac{\partial}{\partial r} \left( \rho A Y_k V_k \right) + A \omega_k W_k \quad (k = 1, 2, ..., K) \]  

Energy equation:

\[ 0 = \frac{1}{c_p} \frac{\partial}{\partial r} \left( \lambda A \frac{\partial T}{\partial r} \right) - \frac{A}{c_p} \sum_{k=1}^{K} \rho Y_k V_k c_{pk} \frac{\partial T}{\partial r} - \frac{A}{c_p} \sum_{k=1}^{K} \omega_k h_k W_k - \frac{A}{c_p} q_{rad} \quad (A = 4\pi r^2) \]  

where \( \rho, c_p, \lambda, T, r, q_{rad}, \) and \( K \) are mass density, heat capacity at constant pressure, thermal conductivity of mixture, temperature, radius, radiative heat loss per unit volume, and the number of species, respectively. \( Y_k, V_k, \omega_k, W_k, c_{pk}, h_k \) are mass fraction, diffusion velocity, net chemical production rate, molecular weight, heat capacity at constant pressure, specific enthalpy of the \( k \)th species, respectively.

Optically thin radiation model (OTM) was adopted to estimate radiative heat loss [4]. Radiative heat loss per unit volume is modeled by the following equation:

\[ q_{rad} = 4\sigma a_p \left( r^4 - T_0^4 \right) \]  

where \( \sigma, a_p, \) and \( T_0 \) are Stefan-Boltzmann constant, Planck mean absorption coefficient, and ambient temperature, respectively. In the present study, pressure is fixed to the atmospheric pressure and \( T_0 \) is fixed to 300 K.

The radiation fraction of counterflow flame, \( r_f \), is defined by the following equation:

\[ r_f = \frac{\int_{-L/2}^{L/2} q_{rad} \, dx}{\int_{-L/2}^{L/2} \sum_{k=1}^{K} \omega_k h_k W_k \, dx} \]  

where, \( L \) is the computation distance, 10 cm.

Xe and Kr were selected as inert gas in the present computation to obtain low-Lewis-number mixture. The ratio of oxidizer mole fraction to inert mole fraction, \( Z \), is fixed to 0.141. A detailed reaction mechanism which consists of GRI-Mech 3.0 without N reaction and inert (37 species, 221 reactions) was adopted. Reaction data of Xe and Kr were used that of Ar in GRI-Mech 3.0. Thermodynamic data of Xe and Kr were obtained from NIST chemistry webbook [5]. Transport data of Xe and Kr were obtained from W.J. Moore’s data [6]. However, polarizability of Kr was obtained from K. Ohno’s data [7]. Thermodynamic and transport data were translated to CHEMKIN format using CHEMKIN 3.7 FITDAT program.

### 3 Computational results

Figure 1 shows computational stretch rates at extinction limit of CH\(_4\)/O\(_2\)/Xe and CH\(_4\)/O\(_2\)/Kr counterflow premixed flames. When equivalence ratio was fixed, two extinction limits at high and low stretch rates were obtained in equivalence ratio within the ranges from 0.50 to 0.37 for Xe, and from 0.50 to 0.42 for Kr. C-shaped extinction limit curves were formed for both flames. Figure 2 shows maximum temperature and radiation fraction at \( \phi = 0.50 \), which corresponds to \( Le \approx 0.5 \) in CH\(_4\)/O\(_2\)/Xe mixture and \( Le \approx 0.7 \) in CH\(_4\)/O\(_2\)/Kr mixture, respectively. Maximum temperature decreased with a decrease of stretch rate in stretch rate lower than around 70 s\(^{-1}\) for Xe and 50 s\(^{-1}\) for Kr. Maximum temperature decreased with an increase of stretch rate in stretch rate higher than around 70 s\(^{-1}\) for Xe and 50 s\(^{-1}\) for Kr. Radiation fraction increased with the decrease of stretch rate in almost all stretch rates. Therefore, extinction limit at higher stretch rate is stretch extinction limit, and the other is radiative extinction limit. However, radiation fraction decreased with the decrease of stretch rate close to the radiative extinction limit.
Figure 3 shows computational flame ball diameters of CH\textsubscript{4}/O\textsubscript{2}/Xe and CH\textsubscript{4}/O\textsubscript{2}/Kr mixtures at $\phi=0.50$. Flame ball diameters decreased with a decrease of CH\textsubscript{4} mole fraction. The extinctions of flame balls were observed. The obtained CH\textsubscript{4} mole fraction at the extinction limits were 0.020 for Xe and 0.027 for Kr.

Flammable region of CH\textsubscript{4}/O\textsubscript{2}/Xe counterflow premixed flame was broader than that of CH\textsubscript{4}/O\textsubscript{2}/Kr counterflow premixed flame. At the same stretch rate, maximum temperature and radiation fraction of CH\textsubscript{4}/O\textsubscript{2}/Xe counterflow flame were higher than those of CH\textsubscript{4}/O\textsubscript{2}/Kr counterflow flame, respectively. Flammable region of CH\textsubscript{4}/O\textsubscript{2}/Xe flame ball was broader than

Figure 1. Computational stretch rates at extinction limit of CH\textsubscript{4}/O\textsubscript{2}/Xe and CH\textsubscript{4}/O\textsubscript{2}/Kr counterflow premixed flames at $Z=0.141$.

Figure 2. Computational maximum temperature and radiation fraction of CH\textsubscript{4}/O\textsubscript{2}/Xe and CH\textsubscript{4}/O\textsubscript{2}/Kr counterflow premixed flames at $\phi=0.50$ and $Z=0.141$. Left: Maximum temperature. Right: Radiation fraction.

Figure 3. Computational CH\textsubscript{4}/O\textsubscript{2}/Xe and CH\textsubscript{4}/O\textsubscript{2}/Kr flame ball diameters at $\phi=0.50$. The extinctions of flame balls were observed. The obtained CH\textsubscript{4} mole fraction at the extinction limits were 0.020 for Xe and 0.027 for Kr.
that of CH₄/O₂/Kr flame ball. Lewis number of CH₄/O₂/Xe mixture is lower than that of CH₄/O₂/Kr mixture. The stronger intensification of flame because of lower Lewis number mixture seems to enable the flammable region to be larger.

4 Recent experimental results

To examine the correlations between flame ball and radiative extinction characteristics of low-stretched counterflow flame which was suggested by numerical simulation, microgravity experiments were conducted very recently using parabolic flight of airplane operated by DAS, Nagoya, Japan.

Using CH₄/O₂/Xe mixture at Z=0.141 and stretch rate of 3 s⁻¹ while equivalence ratio decreases from 0.63 to 0.30, the formation of a ball-like flame after the extinction of counterflow planar flames was observed at the stagnation position. Figure 4 shows the flame images of near-limit planar flame and the ball-like flame. The transition of flame shape was observed around 0.4. The formed ball-like flame immediately moved outward along counterflow streamline.

The present computation showed that the radiative extinction of CH₄/O₂/Xe counterflow premixed flame at 0.37 occurred at 5 s⁻¹. However, the flame ball solution, that is to say, the steady flame solution in stationary, namely non-stretched, mixture was obtained at the same equivalence ratio. It seems that around 0.4, the radiative extinction of low-stretched counterflow flame and the formation of a ball-like flame occurred. And it seems that the formed ball-like flame moved outward because the mixture was not completely stationary.

5 Conclusions

From the numerical simulations of CH₄/O₂/Xe and CH₄/O₂/Kr and experiments in microgravity using CH₄/O₂/Xe counterflow premixed flame, these conclusions were obtained.
1. CH₄/O₂/Xe premixed counterflow flame had a larger flammable region than CH₄/O₂/Kr premixed counterflow flame at φ=0.50 and Z=0.141.
2. CH₄/O₂/Xe flame ball had a larger flammable region than CH₄/O₂/Kr flame ball at φ=0.50.
3. The extension of flammable region of CH₄/O₂/Xe flame compared to CH₄/O₂/Kr flame is due to lower Lewis number of CH₄/O₂/Xe mixture than that of CH₄/O₂/Kr mixture.
4. At the stretch rate of 3 s⁻¹, the transition from CH₄/O₂/Xe counterflow flames to a ball-like flame was observed. However, the formed ball-like flame moved outward along counterflow streamline.

References