Outwardly Propagating Spherical Flames with Thermally Sensitive Intermediate Kinetics and Radiative Loss

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1 Introduction

Due to the simple flame configuration and well-defined flame stretch rate, the outwardly propagating spherical flame (OPF) method is one of the most favorable methods to measure the laminar flame speed and Markstein length [1]. In the literature, OPF was been extensively studied by using asymptotic techniques. For example, Ronney and Sivashinsky [2] investigated the effects of radiative loss on spherical flame propagation and extinction; Bechtold *et al.* [3] assessed the impact of radiative loss on self-extinguishing flames and self-wrinkling flames; He [4] and Chen and Ju [5] developed theory on spherical flame initiation and propagation; and Chen *et al.* [6] studied the effects of radiation on the flame propagation speed and Markstein length. However, in all the studies [2-6] mentioned above, one-step, irreversible, global reaction model was employed. In such a one-step model the fuel is converted directly into products and heat, and thus the role of energetic active radicals is not considered [7]. Numerous elementary reactions related to fuel and reactive intermediate species appear in practical combustion of hydrocarbon fuels [8]. As such, flame propagation is not only influenced by properties of fuel, but also by those of intermediate species (especially radicals involved in chain branching reactions). In order to achieve more essential understanding of spherical flame propagation, chain-branching kinetics of intermediate species should also be considered.

Recently, Dold and coworkers [7, 9-11] proposed the following simplified version of the Zel'dovich-Liñán model

$$F + Z \rightarrow 2Z$$
 : $k_B = A_B \exp(-T_B/T)$ (1a)

$$Z + M \to P + M \qquad : \qquad k_C = A_C \tag{1b}$$

where F, Z, and P denote fuel, radical, and product, respectively. This model involves a thermally sensitive chain branching reaction (1a) with a rate constant k_B in Arrhenius form (A_B and T_B are the frequency factor and activation temperature, respectively) and a completion reaction (1b) with a rate constant k_C which is equal to the frequency factor A_C and is independent of temperature T. Based on this model, the structure and stability of non-adiabatic flame balls and propagating planar flames were investigated [7, 9-11]. The simplified Zel'dovich-Liñán model was also utilized by Gubernov and coworkers [12, 13] in their studies on the kinetic characteristics of flame extinction. Recently, this model was employed to study the adiabatic spherical flame initiation and propagation [14]. It was found that spherical flame initiation and propagation are strongly affected by the Lewis numbers of fuel and radical as well as the heat of reaction [14].

In this study, a general correlation between flame speed and flame radius of OPF with thermal sensitive intermediate kinetics and radiative loss will be derived first. Based on this correlation, the effects of Lewis numbers of fuel and radical species as well as radiative heat loss on the propagation speed of OPF will be assessed. Moreover, the effects of fuel Lewis number, radical Lewis number, and radiative loss intensity on Markstein length are discussed.

2 Mathematical Model

By adopting constant thermal properties, infinite large activation energy, quasi-steady, and quasiplanar assumptions [4-6, 15, 16,], the dimensionless conservative equations for fuel and radical mass fractions, as well as temperature are given as

$$\frac{d^2 Y_F}{d\xi^2} + \left(ULe_F + \frac{2}{R}\right)\frac{dY_F}{d\xi} = 0$$
(2a)

$$\frac{d^2 Y_Z}{d\xi^2} + \left(ULe_Z + \frac{2}{R}\right)\frac{dY_Z}{d\xi} - Le_Z Y_Z = 0$$
(2b)

$$\frac{d^2T}{d\xi^2} + \left(U + \frac{2}{R}\right)\frac{dT}{d\xi} + QY_z - l = 0$$
(2c)

where $\xi(=r-R)$, Y_F , Y_Z , T are scaled radial coordinate, fuel mass fraction, radical mass fraction, and temperature, respectively. The variables U (=dR/dt) and R are the spherical flame propagation speed and flame radius, respectively. The dimensionless heat release Q signifies the total chemical enthalpy of the premixture, and l the dimensionless rate of radiative heat loss (here we model it as l=hT, the constant h is termed as heat-loss intensity [10]). Le_F and Le_Z are the fuel and radical Lewis number, respectively.

Equations (2a-2c) can be solved analytically subject to the following boundary conditions at unburned zones ($\xi \rightarrow +\infty$) and burned zones ($\xi \rightarrow -\infty$)

$$\xi \to +\infty, T = 0, Y_F = 1, Y_Z = 0$$
 (3a)

$$\xi \to -\infty, dT/d\xi = dY_F/d\xi = dY_Z/d\xi = 0$$
 (3b)

and the jump conditions at the flame front (ξ =0) [7, 9-11]

$$[Y_F] = [Y_Z] = [T] = T - 1 = \left[\frac{dT}{d\xi}\right] = \left[\frac{1}{Le_F}\frac{dY_F}{d\xi} + \frac{1}{Le_Z}\frac{dY_Z}{d\xi}\right] = Y_F\frac{dT}{d\xi} = 0$$
(4)

The exact distributions of fuel and radical mass fractions and temperature can be obtained analytically and is not presented here due to space limitation. The general correlation between flame velocity U and flame radius R is derived as

$$\lambda_{1} + \frac{QY_{Z0}(\lambda_{1} - \gamma_{1})}{\gamma_{1}^{2} + (U + 2/R)\gamma_{1} - h} = \lambda_{2} + \frac{QY_{Z0}(\lambda_{2} - \gamma_{2})}{\gamma_{2}^{2} + (U + 2/R)\gamma_{2} - h}$$
(5)

where $Y_{Z0} = Le_Z \left(U + 2/RLe_F\right) / (\gamma_1 - \gamma_2)$, $\gamma_{1,2} = -0.5 \left(ULe_Z + 2/R\right) \pm 0.5 \sqrt{\left(ULe_Z + 2/R\right)^2 + 4Le_Z}$, and $\lambda_{1,2} = -0.5 \left(U + 2/R\right) \pm 0.5 \sqrt{\left(U + 2/R\right)^2 + 4h}$. With the help of this correlation, the effects of Le_F , Le_Z , and h on OPF and the Markstein length can be assessed and are presented in the following section.

3 Results and Discussions

The normalized flame velocities as functions of flame radii and normalized stretch rates with variable Lewis numbers of fuel and intermediate species are plotted in Fig. 1. Here Q=2.0, h=0, and U^0 corresponds to flame speed at zero stretch rate. Figure 1(a) shows that the U-R curves of OPF are

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strongly affected by Le_F and Le_Z . For three curves with $Le_Z=1.0$, U first increases and then slightly decreases with increased R for $Le_F=0.5$, while U rises monotically as R increases for $Le_F=1.0$ and 2.0. For curves with $Le_F=1.0$, the OPF trajectories are appreciably changed for variations of Le_Z (0.5, 1.0, and 1.5). The present results are consistent with those with one-step [4-6] and two-step chemistry [14]. Fig. 1(b) shows the dependence of normalized flame speeds on normalized flame stretch rates with Q=2.0 and h=0. For OPF, flame stretch rate is K=2U/R, and the Markstein length, L, is defined as the slope in U-K plot when K approaches zero [6]. It is seen from Fig. 1(b) that the Markstein length, L, is strongly affected by Lewis numbers of fuel and radical.



Figure 1. Normalized spherical flame propagation speed as functions of (a) flame radius and (b) normalized stretch rate with variable Lewis numbers of fuel and radical at Q=2.0 and h=0.



Figure 2. Spherical flame propagation speed as functions of (a) flame radius and (b) normalized stretch rate with variable heat-loss intensities at Q=2.0, $Le_F=1.0$ and $Le_Z=1.0$.

Figure 2 demonstrates effects of radiation on OPF. It is noted that there are two solutions for radiative flames and only the fast-stable solution is presented in Fig. 2. At the same flame radius R, Fig. 2(a) shows the flame propagation speed, U, decreases with the heat-loss intensity, h. However, Fig. 2(b) shows the Markstein length, L, increases with the heat-loss intensity, h.

Figure 3 shows the effects of Le_F , Le_Z and h on the Markstein length, L. According to Fig. 3(a), the Markstein length increases monotonically with the fuel Lewis number For OPF (positively stretched flame), the difference between the enthalpy gain (due to fuel diffusion into the flame) and heat loss (due to thermal conduction away from the flame) increases with Le_F since Le_F is the ratio between fuel mass diffusivity and thermal diffusivity [14]. Therefore, the larger the fuel Lewis number, the stronger the influence of stretch on spherical flame propagation, and thus the larger the Markstein length [17, 18]. Fig. 3(b) shows that the Markstein length monotonically decreases with the radical Lewis number.

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This is due to the fact that the radical diffuses out of the reaction zone while fuel diffuses into it. For OPF with positive stretch, the larger the radical Lewis number, the smaller the mass diffusivity of the radical, and the less the radical enthalpy diffused away from the reaction zone [14]. Consequently, at a given fuel Lewis number, the positively stretched flame becomes stronger for a larger radical Lewis number. Fig. 3(c) shows that the Markstein lengt changes with heat-loss intensity at different Lewis numbers. When Lewis numbers of fuel and radical equal to unity, the Markstein length slightly increases as *h* successively become large from 0 to 0.7. However, for cases with $Le_F=2.0$, $Le_Z=1.0$ and $Le_F=1.0$, $Le_Z=0.5$, the extend to which heat-loss intensity *h* affects the Markstein length *L* is more pronounced than that for case with $Le_F=Le_Z=1.0$, and *L* increases sharply when *h*>0.05. As such, the Markstein length *L* strongly depends on radiative heat-loss intensity *h*.



Figure 3. The dependence of Markstein length on (a) fuel Lewis number, (b) radical Lewis number, and (c) heat-loss intensity.

4 Conclusions

The outwardly propagating spherical flames (OPF) with thermally sensitive intermediate kinetics and radiative loss are asymptotically investigated in the present study. The theoretical correlation describing flame propagating velocity and flame radius of large-flame-radius OPF is derived, which includes Lewis numbers of fuel and radical species, heat release and radiative heat loss. The effects of Lewis numbers of fuel and radical as well as radiative heat loss on OPF and the Markstein length are examined. It is found that OPF is strongly influenced by the fuel Lewis number, radical Lewis number and radiative heat loss, while decreases with the radical Lewis number.

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