Effects of Endothermic Chain-branching Reaction on Spherical Flame Initiation and Propagation

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1 Introduction

Due to its simple one-dimension configuration, spherical flame has been popularly used to study the initiation and propagation of premixed flames. Usually, one-step irreversible global reaction model is used in theoretical analysis of spherical flame. However, 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. Recent studies [1-3] indicated that premixed flame initiation and propagation are affected by the transport and chemical properties of intermediate species. In these studies, the two-step chain-branching model proposed by Dold [4] was used. This model is the simplified version of Zel'dovich-Liñán model. It comprises a chain branching reaction F+Z→2Z, and a recombination reaction Z+M→P+M, where F, Z, and P represent fuel, radical, and product, respectively, and M denotes any type of molecule. The branching reaction is thermally sensitive and has a rate constant depending on the temperature in the Arrhenius form, while the rate of the recombination reaction is independent of the temperature. In previous studies [1-4], the chain-branching reaction is assumed to be thermally neutral and thereby the completion reaction releases all the heat. However, in practical combustion of hydrocarbon fuels, the chain-branching reaction is usually endothermic rather than thermally neutral [4]. Currently, it is not clear how the endothermicity of the chain-branching reaction affects premixed flame initiation and propagation. This motivates the present work, which aims to answer this question.

In this study, a theoretical model containing endothermic chain-branching reaction and exothermic recombination reaction is used to analyze spherical flame initiation and propagation. The simplified Zel'dovich-Liñán model is used. Unlike previous studies, we consider the endothermicity of the chain-branching reaction. Within the framework of large activation energy and quasi-steady assumptions, the analytical solutions for the distributions of fuel mass fraction, radical mass fraction and temperature are obtained and a correlation describing spherical flame propagation is derived. Based on the correlation, the effects of endothermic chain-branching reaction on stretched spherical flame propagation speed, Markstein length, unstretched planar flame speed, ignition kernel development and critical ignition conditions are examined.

2 Theoretical analysis

The simplified Zel'dovich-Liñán model proposed by Dold and coworkers is employed in this theoretical analysis[4]. Unlike previous studies [1-4], here we consider the endothermicity of the chain-branching reaction. One-dimensional spherical flame initiation is considered and the mathematical model is similar to that in Refs. [1, 2]. The constant density and quasi-steady assumptions [6-9] are employed. In the coordinate attached to the propagating flame front and under the assumption of large activation energy, the non-dimensional governing equations for temperature, T, and mass fractions of fuel, Y_F, and radical, Y_Z, in the unburned and burned zones are [1, 2]

$$-U\frac{dY_F}{dr}=\frac{1}{Le_F}\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dY_F}{dr}),\ -U\frac{dY_Z}{dr}=\frac{1}{Le_Z}\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dY_Z}{dr})-\Lambda Y_Z\ ,\ -U\frac{dT}{dr}=\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dT}{dr})+Q_C\Lambda Y_Z \quad (1)$$

$$\Lambda Le_Z=(1+\frac{1-T_C}{Q})(S_2^2-S_2)(S_1-S_2),S_{1,2}=\frac{Le_Z\pm\sqrt{Le_Z{}^2+4\Lambda Le_Z}}{2} \quad (2)$$

where r is the non-dimensional radial coordinate. Le_F and Le_Z are the Lewis numbers of the fuel and radical, respectively. U is propagation speed of the flame front, Q_C is the specific heat release of the completion reaction. Λ is the eigenvalue related to the flame speed [5] and is given by equations (2) implicitly.The non-dimensional procedure is the same as that in [5] and thereby it is not repeated here.

In this study, the impact of external energy deposition on spherical flame initiation and propagation is investigated and the ignition energy is provided as a heat flux at the center. Steady-state energy deposition is employed in order to achieve an analytical solution [6],

$$r\to 0:\quad r^2\frac{\partial T}{\partial r}=-q\ ,\ \frac{\partial Y_F}{\partial r}=0,\ \frac{\partial Y_Z}{\partial r}=0\ ,\ r\to\infty:\quad T=0,\quad Y_F=1,\ Y_Z=0 \quad (3)$$

where q is the ignition power normalized by $4\pi\lambda r_s T_s$.

In the asymptotic limit of high activation energy ($\beta\to+\infty$), chemical reactions are confined at an infinitesimally thin flame sheet ($r=R$), so the reaction zone for the chain-branching reaction can be replaced to leading order by a reaction sheet or surface across which suitable jump conditions apply, and such that no chain-branching reaction or heat release occurs on either side of this reaction sheet (i.e. ω=0). The conditions at the flame front ($r=R$) are [4]

$$[Y_F]=[Y_Z]=[T]=\left[\frac{1}{Le_F}\frac{\partial Y_F}{\partial r}+\frac{1}{Le_Z}\frac{\partial Y_Z}{\partial r}\right]=T-T_C=Y_F\frac{\partial T}{\partial r}=0,\ [\frac{\partial T}{\partial r}]=\frac{Q_B}{Le_F}[\frac{\partial Y_F}{\partial r}] \quad (4)$$

where $[f]=f[r=R^+]-f[r=R^-]$. It is noted that here Q_B denotes the endothermicity of the chain-branching reaction. The global heat release Q is the difference between Q_C and Q_B.

Equations (1) can be solved analytically in the burned and unburned zones respectively, and the exact solutions for mass concentration, radical concentration and temperature are:

$$Y_F(r)=\begin{cases}0 & if\quad 0\le r\le R\\ 1-\dfrac{\int_r^\infty \xi^{-2}e^{-Le_F U\xi}d\xi}{\int_R^\infty \xi^{-2}e^{-Le_F U\xi}d\xi} & if\quad r\ge R\end{cases} \quad (5)$$

$$Y_Z(r)=\begin{cases}Y_{Zf}\exp[0.5(ULe_Z+k)(R-r)]\dfrac{F(kr,ULe_Z/k,-ULe_Z/k)}{F(kR,ULe_Z/k,-ULe_Z/k)} & if\quad 0\le r\le R\\ Y_{Zf}\exp[0.5(ULe_Z+k)(R-r)]\dfrac{G(-kr,ULe_Z/k,-ULe_Z/k)}{G(-kR,ULe_Z/k,-ULe_Z/k)} & if\quad r\ge R\end{cases} \quad (6)$$

$$T(r)=\begin{cases} T_C+\int_r^R\int_0^s I(s,\xi)d\xi ds+q\int_r^R s^{-2}e^{-Us}ds \quad if \quad 0\le r\le R \\ [T_C+\int_R^\infty\int_s^\infty I(s,\xi)d\xi ds]\dfrac{\int_r^\infty s^{-2}e^{-Us}ds}{\int_R^\infty s^{-2}e^{-Us}ds}-\int_r^\infty\int_s^\infty I(s,\xi)d\xi ds \quad if \quad r\ge R \end{cases} \tag{6}$$

where

$$F(a,b,c)=\int_0^1 e^{at}t^b(1-t)^c\mathrm{d}t, G(a,b,c)=\int_0^\infty e^{at}t^b(1+t)^c\mathrm{d}t$$

$$k=\sqrt{(ULe_Z)^2+4\Lambda Le_Z}$$

$$Y_{Zf}=\frac{Le_Z Le_F{}^{-1}k^{-1}R^{-2}e^{-Le_F UR}/\int_R^\infty \xi^{-2}e^{-Le_F U\xi}d\xi}{\dfrac{F(kR,1+ULe_Z/k,-ULe_Z/k)}{F(kR,ULe_Z/k,-ULe_Z/k)}+\dfrac{G(-kR,1+ULe_Z/k,-ULe_Z/k)}{G(-kR,ULe_Z/k,-ULe_Z/k)}}$$

$$I(s,\xi)=(\frac{\xi}{s})^2 e^{-U(s-\xi)}Q_C\Lambda Y_Z(\xi)$$

Substituting the temperature distribution into the jump condition, we obtain the following correlation depicting the change of the flame propagation speed U with the flame radius R:

$$\int_R^\infty\int_0^s I(s,\xi)d\xi ds+q\int_R^\infty s^{-2}e^{-Us}ds-\frac{Q_B}{Le_F}e^{UR(1-Le_F)}\frac{\int_R^\infty s^{-2}e^{-Us}ds}{\int_R^\infty s^{-2}e^{-Le_F Us}ds}=1 \tag{7}$$

By numerically solving Eq. (7), the results for spherical flame initiation and propagation can be obtained and the effects of endothermic chain-branching reaction can be examined by changing the value of Q_B.

3 Results and discussion

We first study the spherical flame propagation without ignition power deposition at the center (q=0). Figure 1 shows the results for mixtures with Le_Z =1, Q=6,T_C=4 and different values of Q_B and Le_F. In Fig. 1(a), solutions on the horizontal axis with U=0 correspond to flame balls, those on the right vertical axis at R=10^3 correspond to planar flames, and those between them represent the propagating spherical flames. Flame propagation speed increases with the flame radius due to the transition from purely diffusion-controlled flame ball to convection-diffusion controlled propagating spherical flame. It is seen that the flame ball radius increases with endothermicity Q_B while the normalized planar flame speed decreases with Q_B. For propagating flames, the U-R curve is shifted toward the right side as the endothermicity Q_B increases. In the two-step chemical model, the endothermicity reduces the rate of the chain branching reaction and thus reduces the production rate of radical. Since the rate of the completion reaction is proportional to the radical concentration, it also decreases as the endothermicity Q_B increases. Consequently, the flame propagation speed decreases with Q_B.

Figure 1(b) shows the stretched flame speed changes linearly with the stretch rate, $K=2U/R$. Consequently, the unstretched flame speed, U^0, and Markstein length, L, can be obtained from linear extrapolation. The results are plotted in Figure 2. As expected, U^0 is shown to decreases as the endothermicity Q_B increases. Moreover, it is seen that the Markstein length L increases monotonically with Q_B. For Q_B=0, the present result the same as that reported in [1] which considered thermally neutral chain-branching reaction. When the chain-branching reaction becomes endothermic, the flame becomes weaker since the radical is more slowly produced and consumed. Usually, weaker flame is more sensitive to the stretch rate [7]. Therefore, the Markstein length becomes larger as the endothermicity Q_B of the chain-branching reaction increases. It is also observed that the effects of endothermicity becomes stronger at higher fuel Lewis number Le_F, lower radical Lewis number Le_Z, or lower crossover temperature T_C. This is due to the facts that 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, the enthalpy loss (due to radical diffusion away from the flame) and heat gain (due to thermal conduction into the flame) increases with Le_Z, and the chain branching reaction rate increases with T_C according to the Arrhenius law. Consequently, higher Le_F, lower Le_Z or lower T_C corresponds weaker flame, on which endothermic reaction has stronger influence.

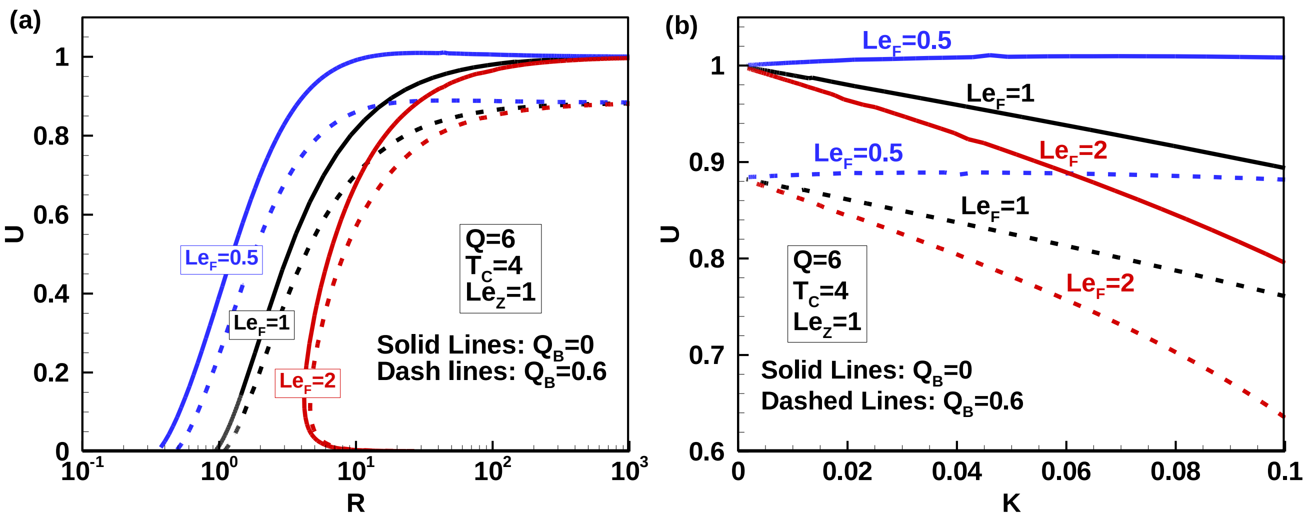

Figure 1 Spherical flame propagation speed as a function of (a) flame radius and (b) stretch rate for Q=6, T_C=4, Le_Z=1.

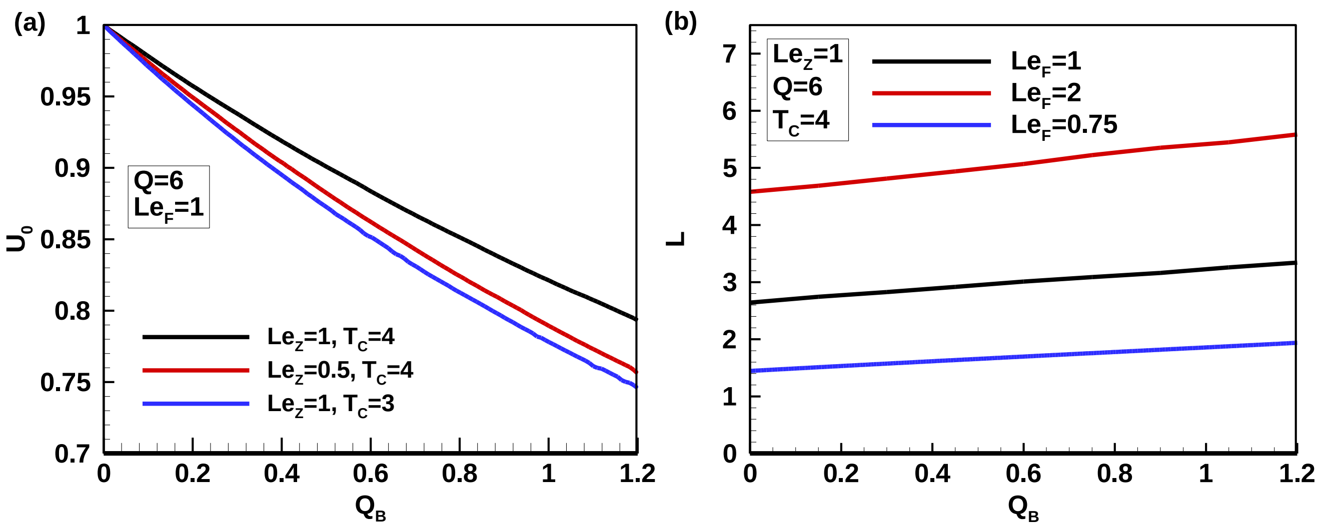

Figure 2 Dependence of (a) unstretched flame speed and (b) Matkstein length on the endothermicity of the chain-branching reaction

Then we consider the case in which an external energy flux (q>0) is deposited in the center of a quiescent pre-mixture. Figure 3 shows the results for Le_Z =1, Q=6, T_C=4, Q_B=0.6, for Le_Z =1, Q=6, T_C=4, Q_B=0.6, (a) Le_F=1 and (b) Le_F=2. The *U-R* curve is the same as that in Fig. 1(a) for the case of q=0, for which the outwardly propagating spherical flame only exists beyond a finite flame radius, which is the flame ball radius *Rz*. When an external energy is deposited at the center, the flame propagation trajectory is changed. At low ignition powers 0<q<q_C, there exists two branches of solutions, the original travelling branch is shifted to the left side and a new branch (ignition kernel) at small radius is formed. With the ignition power increases, two branches approaches and finally merges. An outwardly propagating spherical flame can be successfully initiated via flame transition along the merged line. Qualitatively, the above results are similar to those for the case of thermal neutral chain-branching reaction as reported in [1]. However, the critical ignition power is affected by the endothermicity of the chain-branching reaction.

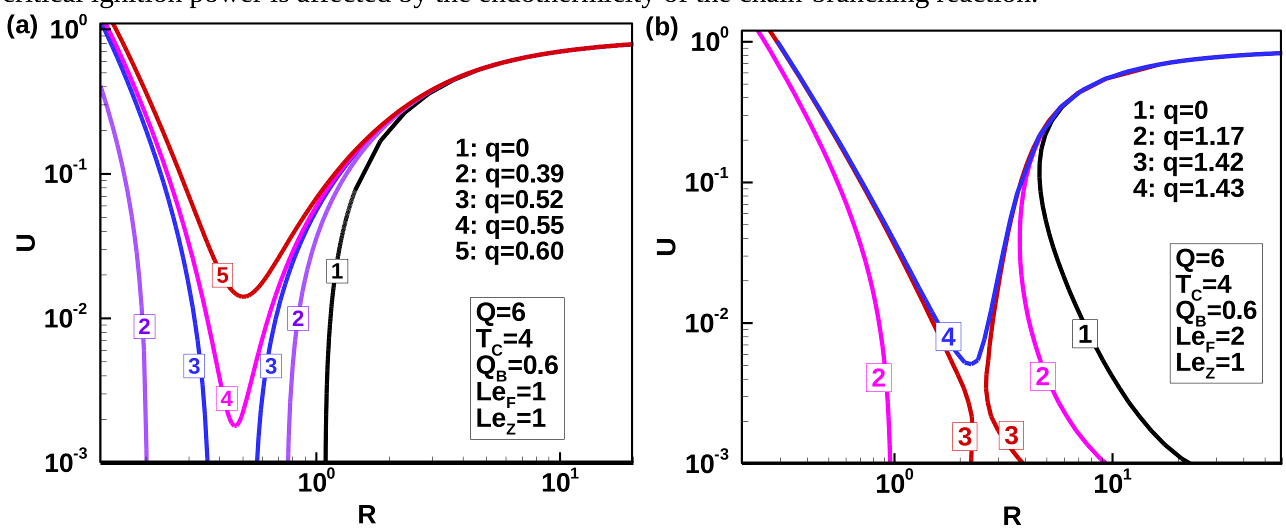

Figure 3 Flame propagation speed as a function of flame radius at different ignition power for Le_Z =1, Q=6, T_C=4, Q_B=0.6, (a) Le_F=1 and (b) Le_F=2

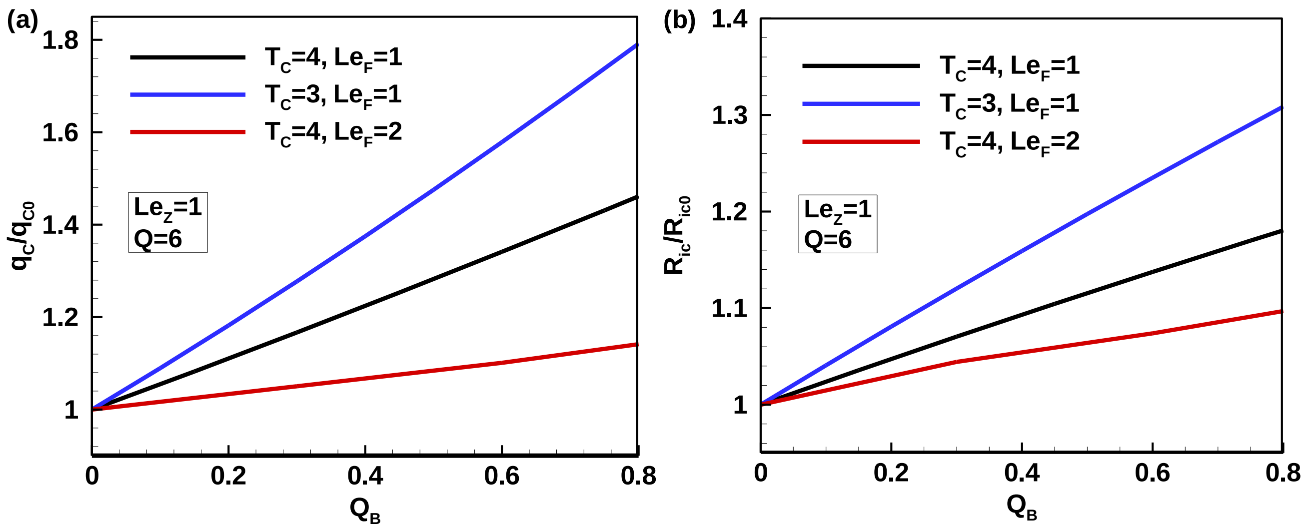

Figure 4 Change of (a) the critical ignition power and (b) the critical ignition radius with the endothermicity of the chain-branching reaction

When $(Le_F+Q_B)<Q_C$, the critical conditions for spherical flame initiation can be determined by analysis on flame ball with energy deposition. The critical ignition power q_C and critical ignition radius R_{iC}, can be determined by the flame ball solution according to $dq/dR=0$. When $(Le_F+Q_B)\geqslant Q_C$, the critical conditions for spherical flame initiation are determined by $R_{iC} = R_C^+=R_C^-$, where R_C^+ is the minimum flame radius of the left branch and R_C^- is the minimum flame radius of the right branch. Figure 4 shows the effects of endothermic reaction on spherical flame initiation. It is seen that the critical ignition power, q_C, and the critical ignition radius, R_{iC}, both increase monotonically with Q_B. Therefore, the endothermicity of the chain-branching reaction inhibits the ignition process. This is expected since the flame becomes weaker and the radical is more slowly produced and consumed as the chain-branching reaction becomes endothermic. Moreover, weaker flame is more sensitive to endothermic reaction and thereby the slope of lines in Fig. 4 is larger at lower crossover temperature or lower fuel Lewis number.

4 Conclusions

The effects of endothermic chain-branching reaction on spherical flame initiation and propagation are studied theoretically using the thermally sensitive intermediate kinetics. Under the large-activation-energy and quasi-steady asusmption, the spatial distributions of fuel and radical concentration, temperature, and the correlation describing spherical flame propagation are derived. Based on this correlation, the effects of endothermic chain-branching reaction are assessed. As the endothermicity of the chain-branching reaction increases, the flame propagation speed decreases while the Markstein length increases, indicating that the stretched flame is more sensitive to stretch rate. As for the ignition process, the critical ignition power and the critical ignition radius both increase monotonically with the the endothermicity of the chain-branching reaction. Therefore, the endothermicity of the chain-branching reaction inhibits the ignition process. For both premixed spherical flame propagation and initiation, the effects of endothermicity become stronger for weaker flames.

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