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Spherical flame initiation and propagation with thermally sensitive intermediate kinetics

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ABSTRACT

Spherical flame initiation and propagation with thermally sensitive intermediate kinetics are studied analytically within the framework of large activation energy and quasi-steady assumptions. A correlation describing different flame regimes and transitions among the ignition kernels, flame balls, propagating spherical flames, and planar flames is derived. Based on this correlation, spherical flame propagation and initiation are then investigated. The flame propagation speed, Markstein length, and critical ignition power and radius are found to strongly depend on the Lewis numbers of fuel and radical and the heat of reaction. For spherical flame propagation, the trajectory is shown to change significantly with the fuel Lewis number and a C-shaped solution curve of flame propagation speed as a function of flame radius is observed for large fuel Lewis numbers. The Markstein length is shown to increase/decrease monotonically with the fuel/radical Lewis number. The influence of stretch on flame propagation (i.e. the absolute value of Markstein length) is found to decrease with the heat of reaction. For spherical flame initiation, the critical ignition power and radius are shown to increase with the fuel Lewis number and to decrease with the radical Lewis number and heat of reaction. Three different flame initiation regimes are observed and discussed. Furthermore, the validity of theoretical prediction is confirmed by transient numerical simulations including thermal expansion and detailed chemistry.

1. Introduction

Flame initiation and propagation are the most fundamental problems in combustion research. Understanding flame initiation and propagation are important for fire safety control and for the development of high-efficiency, low-emission combustion engines. Since spherical flame has the simplest geometry, spherical flame initiation and propagation have been extensively studied via theoretical analysis [1–21].

Spherical flame initiation was first investigated based on the thermal theory [1–3]. The quenching distance or flame thickness was considered to be the critical length controlling spherical flame initiation. However, fuel consumption and thus mass diffusion were not considered in the thermal theory [1–3]. A more accurate description of flame initiation was proposed later by Zel'dovich based on studies of adiabatic flame balls [3]. Since the adiabatic flame balls were found to be inherently unstable: a small perturbation will cause the flame either to propagate inward and eventually extinguish or to propagate outward and evolve into a planar flame [4], the flame ball radius was considered to be the critical length controlling spherical flame initiation [3–5]. Recently, He [8] found that flame initiation for mixtures with large Lewis numbers was controlled not by the radius of stationary flame ball but by a minimum flame radius for the existence of self-sustained propagating spherical flames. Chen and coworkers [10,11] showed that spherical flame initiation was strongly affected by the fuel Lewis number as well as the radiative loss.

Spherical flame propagation has also been extensively studied by using asymptotic techniques. For examples, Frankel and Sivashinsky [12] examined the thermal expansion effect and Lewis number effect on propagating spherical flames; Chung and Law [13] conducted integral analysis for propagating spherical flames; Bechtold and coworkers [14–17] studied the hydrodynamic and thermal-diffusion instabilities and effects of radiative loss in self-extinguishing and self-wrinkling flames; Ronney and Sivashisky [18] studied the expanding spherical flames within the framework of a slowly varying flame (SVF) theory; Sung et al. [19] found that positive stretch of expanding flames promotes the onset of flame pulsation; Chen et al. [21] examined the radiative effects on spherical flame propagation speed and Markstein length.

In all the studies [4–21] mentioned above, one-step, irreversible, global reaction model was employed. The popularity of this

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model is partly due to its inherent simplicity. Nevertheless, the one-step model has led to many useful and qualitatively correct predictions for spherical flame initiation and propagation [4–21]. 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 [22]. In practical combustion of hydrocarbon fuels, numerous elementary reactions related to fuel and reactive intermediate species appear [23]. As such, flame initiation and propagation are not only affected 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 flame initiation and propagation, chain branching kinetics of intermediate species should also be considered. However, inclusion of complicated chemistry requires numerical calculations and the results are lack of generality.

A relative simple generalization of the one-step model is provided by the Zel'dovich–Liñán model [3,24]. The model comprises a chain branching reaction $F+Z\rightarrow 2Z$, and a chain-breaking (or recombination) reaction $Z+Z\rightarrow 2P$, where F, Z, and P represent fuel, radical, and product, respectively. This model was used by different researchers in their studies on laminar flames [25–31]. Recently, in seeking simple analytical descriptions, Dold and coworkers [22,32–34] proposed the following simplified version of the Zel'dovich–Liñán model

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

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

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 [22,32–34]. The simplified Zel'dovich–Liñán model was also utilized by Gubernov and coworkers [35,36] in their studies on the kinetic characteristics of flame extinction.

In this study, we will use the simplified Zel'dovich–Liñán model given in Eq. (1) to investigate spherical flame initiation and propagation. The objectives of the present study are twofold. First, we find a general theoretical description of different flame regimes and transitions among the ignition kernels, flame balls, propagating spherical flames, and planar flames. Second, we assess the effects of fuel and radical Lewis numbers and heat of reaction on flame propagation speed, Markstein length, minimum ignition energy, and critical length controlling spherical flame initiation. Compared to the works of Dold and coworkers [22,32–34], the new development of this study is that the simplified Zel'dovich–Liñán model is used to investigate the critical ignition conditions and propagating spherical flames with positive stretch rate. The rest of the paper is organized as follows. The mathematical model is introduced in the next section. In Section 3, analytical solutions for spherical flame initiation and propagation with thermally sensitive intermediate kinetics are presented and validated in limiting cases. Moreover, the effects of fuel and radical Lewis numbers and heat of reaction on spherical flame initiation and propagation are studied. In order to confirm the validity of theoretical prediction, detailed numerical simulations are conducted in Section 4. Finally, the conclusions are presented in Section 5.

2. Mathematical model

Spherical flame initiation and propagation are studied using the classical reactive–diffusive model (constant values for density ρ, specific heat C_P, diffusion coefficients of fuel D_F and radical D_Z, thermal conductivity λ, and heat of reaction Q) [37,38]. Based on the chain branching kinetics, Eq. (1), the one-dimensional conservation equations for temperature, T, and mass fractions of fuel, YF, and radical, YZ, in a spherical coordinate are

$$\rho\frac{\partial Y_F}{\partial t}=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\rho D_F\frac{\partial Y_F}{\partial r}\right)-W_F\omega_B \tag{2a}$$

$$\rho\frac{\partial Y_Z}{\partial t}=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\rho D_Z\frac{\partial Y_Z}{\partial r}\right)+W_Z(\omega_B-\omega_C) \tag{2b}$$

$$\rho C_P\frac{\partial T}{\partial t}=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\lambda\frac{\partial T}{\partial r}\right)+Q\omega_C \tag{2c}$$

where t and r are time and radial coordinate respectively. The reaction rates are [32,33]

$$\omega_B=\frac{\rho Y_F}{W_F}\frac{\rho Y_Z}{W_Z}A_B\exp\left(-\frac{T_B}{T}\right),\quad \omega_C=\frac{\rho Y_Z}{W_Z}\frac{\rho}{W}A_C \tag{3}$$

where W_F and W_Z are the molecular weights of fuel and radical, respectively, and W represents the mean molecular weight.

Since the constant-density model neglects thermal expansion, there is no convective flux in the governing equations. Moreover, the effects of radiative loss on spherical flame initiation and propagation [10,21] are not considered in this study. Different from previous studies considering one-step chemistry [8,10,17], we have the additional equation, Eq. (2b), depicting the radical's production by the chain branching reaction (1a), and consumption by the recombination reaction (1b) as well as the diffusion process.

Following Dold et al. [33], we introduce the non-dimensional variables:

$$t'=\frac{t}{t_s},\quad r'=\frac{r}{r_s},\quad T'=\frac{T-T_0}{T_s},\quad Y_F'=\frac{Y_F}{Y_{F0}},\quad Y_Z'=\frac{Y_Z}{Y_{Zs}} \tag{4}$$

along with the definitions

$$t_s=\frac{r_s^2\rho C_P}{\lambda},\quad r_s^2=\frac{\lambda W}{\rho^2C_PA_C},\quad Y_{Zs}=\frac{W_ZY_{F0}}{W_F},\quad Q'=\frac{QY_{F0}}{C_PT_sW_F},$$
$$\beta=\frac{T_BT_s}{(T_0+T_s)^2},\quad \sigma=\frac{T_s}{T_0+T_s} \tag{5}$$

where T_0 and Y_{F0} are, respectively, the temperature and fuel mass fraction in the fresh mixture. The Zel'dovich number, β, defined in Eq. (5) is based on the reference temperature T_0+T_s instead of the adiabatic flame temperature [22,33]. Following Refs. [22,33], the scaling temperature, T_s, is chosen so that $\omega_B=\beta^2\omega_C$ at the temperature of T_0+T_s, i.e.

$$\frac{A_BW}{A_CW_F}Y_{F0}=\beta^2\exp\left(\frac{T_B}{T_0+T_s}\right) \tag{6}$$

It is noted that unlike the non-dimensional process in Ref. [33], the mass diffusivities of fuel and radical are not used for scaling in Eq. (5). Therefore, the Lewis numbers of fuel, $Le_F=\lambda/(\rho C_PD_F)$, and radical, $Le_Z=\lambda/(\rho C_PD_Z)$, are present in the non-dimensional governing equations, and thus the effects of Le_F and Le_Z on spherical flame initiation and propagation can be assessed in this study.

In the coordinate attached to the moving flame front, $R=R(t)$, the non-dimensional conservation equations take the following form (after dropping the primes) [8,10]

$$\frac{\partial Y_F}{\partial t}-U\frac{\partial Y_F}{\partial r}=\frac{1}{Le_F}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial Y_F}{dr}\right)-\omega \tag{7a}$$

$$\frac{\partial Y_Z}{\partial t}-U\frac{\partial Y_Z}{\partial r}=\frac{1}{Le_Z}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial Y_Z}{\partial r}\right)+\omega-Y_Z \tag{7b}$$