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Effects of Soret diffusion on spherical flame initiation and propagation

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ABSTRACT

Dynamics of spherical flame initiation and propagation with Soret diffusion are investigated using large-activation-energy asymptotic analysis. Under the assumptions of constant density and quasi-steady flame propagation, a general correlation between the flame propagating speed and flame radius considering Soret diffusion and external energy deposition is derived. Emphasis is placed on assessing the effects of Soret diffusion on spherical flame propagation speed, Markstein length, and critical ignition condition. The stretched flame speed is found to be increased and reduced by the Soret diffusion of light and heavy fuels, respectively. For both light and heavy fuels, the absolute value of Markstein length increases after including Soret diffusion, indicating that premixed flames become more sensitive to stretch rate with Soret diffusion. It is found that the Markstein length can be characterized by an effective Lewis number which includes the effects of Soret diffusion. Moreover, Soret diffusion is shown to affect the ignition process since the spherical flame kernel is highly stretched. For large hydrocarbon fuels with high Lewis numbers, the minimum ignition power becomes much larger after considering Soret diffusion.
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1. Introduction

The successful ignition of a static pre-mixture is determined by the evolution of the ignition kernel. The ignition kernel is highly curved and stretched. Its propagation is controlled by the stretch effects coupling with the preferential diffusion between heat and mass (i.e. the Lewis number effect) [1,2]. Therefore, critical ignition condition strongly depends on the Lewis number of the deficient reactant [3–9]. Specifically, due to the high positive stretch rate of the ignition kernel, the minimum ignition energy and critical ignition radius increase significantly with the Lewis number [6–9].

In most of previous studies on ignition and spherical flame propagation, the mass transport was represented by Fickian diffusion (mass diffusion due to concentration gradient) while little attention was paid to Soret diffusion (mass diffusion due to temperature gradient). In the presence of very light or heavy species and steep temperature gradient, Soret diffusion, which drives light (heavy) species toward (away from) the hot zone, is also important for the mass transport [10]. In a spark ignition process, the temperature inside the ignition kernel after spark discharge is very high and thus there exists large temperature gradient. It is therefore expected that ignition and flame kernel propagation are influenced by the Soret diffusion.

In the literature, Soret diffusion in combustion has been mainly studied through numerical simulation. For examples, the Soret diffusion of heavy species such as particle and soot was investigated by Rosner and coworkers [11,12]; the influence of Soret diffusion on flame extinction was analyzed by Ern and Giovangigli [13,14] and Law and coworkers [15,16]; the Soret diffusion effects on laminar flame speed were assessed by Bongers and de Goey [17] and Yang et al. [18]. The readers are referred to Refs. [18,19] for a summary of previous studies on this subject. Recently, Liang et al. [20,21] have examined the Soret diffusion effects on the ignition and propagation of H_2/CO/air flames through numerical simulation with detailed chemistry and transport. It was found that the minimum ignition energy and stretched flame speed are greatly affected by the Soret diffusion [20,21].

The numerical studies [11–21] mentioned above indicated discernable effects of Soret diffusion in combustion with species that are very light or very heavy. Unfortunately, numerical simulation is usually constrained to specific fuel and hence the conclusion is lack of generality. Unlike simulation, theoretical analysis is helpful for general understanding of the physical insight into the problem. However, there are only a few theoretical studies on Soret effects in the literature. Garcia-Ybarra et al. [22,23] studied the Soret diffusion effects on thermo-diffusive stability limits and Markstein lengths of premixed flames. Arias-Zugasti and Rosner [24] assessed

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the influence of Soret diffusion on counterflow diffusion flames. Fong et al. [25] examined the Soret diffusion effects on laminar diffusion flame in high density fluids. In these studies [22–25], only the planar flame was analyzed. However, in the literature there is no theoretical analysis on premixed spherical flame kernel development.

Therefore, the objectives of this study are to provide a theoretical description of premixed spherical flames with Soret diffusion and to assess the effects of Soret diffusion on spherical flame initiation and propagation. In the following, we shall first introduce the theoretical model and derive a correlation describing the spherical flame initiation and propagation with Soret diffusion based on the quasi-steady and large-activation-energy assumptions (the chemical source term is not solved, but is approximated by the corresponding jump conditions across the flame). Then, based on this correlation, we shall examine the effects of Soret diffusion on stretched flame speed, Markstein length, and critical ignition condition.

2. Theoretical analysis

2.1. Mathematical model

Similar to our previous study [6], one-dimensional, adiabatic spherical flame initiation and propagation are considered in the theoretical analysis. Due to its simple geometry and well defined stretch rate, the spherical propagating flame is generally employed to measure the laminar flame speed [26–35], especially at high pressures [36–39]. As shown in Fig. 1, a self-sustained outwardly propagating spherical flame can be established through successful ignition at the center of a quiescent homogeneous combustible mixture. The flame structure consists of a burned gas zone, a thin reaction zone (which is considered as a flame sheet at large-activation energy), and an unburned zone.

One-step, first-order, global reaction model is employed. Therefore, the coupling between Soret diffusion flux and elementary reaction rates [20] is not included in the present model and we focus on the transport effects. The mixture is assumed to be deficient in fuel and thus only fuel concentration needs to be considered. For the sake of simplicity, we employ the diffusive-thermal model [1,40], according to which the density is constant and the flow is static without convection. In a one-dimensional spherical coordinate, the governing equations for temperature $\widetilde{T}$ and fuel mass fraction $\widetilde{Y}$ are

$$\widetilde{\rho}\widetilde{C}_P\frac{\partial \widetilde{T}}{\partial \widetilde{t}}=\frac{1}{\widetilde{r}^2}\frac{\partial}{\partial \widetilde{r}}\left(\widetilde{r}^2\widetilde{\lambda}\frac{\partial \widetilde{T}}{\partial \widetilde{r}}\right)+\widetilde{q}\widetilde{\omega} \tag{1}$$

$$\widetilde{\rho}\frac{\partial \widetilde{Y}}{\partial \widetilde{t}}=-\frac{1}{\widetilde{r}^2}\frac{\partial}{\partial \widetilde{r}}(\widetilde{r}^2\widetilde{j}_Y)-\widetilde{\omega} \tag{2}$$

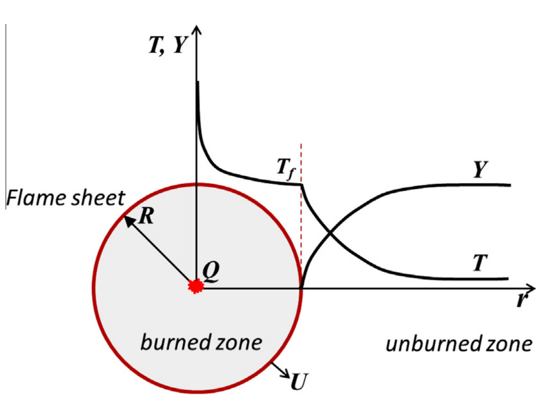

Fig. 1. Schematization of the spherical flame structure.

with

$$\widetilde{\omega}=\widetilde{\rho}\widetilde{A}\widetilde{Y}\exp\left(-\frac{\widetilde{E}}{\widetilde{R}^0\widetilde{T}}\right) \tag{3}$$

where $\widetilde{t}$ and $\widetilde{r}$ are temporal and spatial coordinate, respectively. The density $\widetilde{\rho}$, heat capacity $\widetilde{C}_P$, and heat conductivity $\widetilde{\lambda}$ of the mixture are all assumed to be constant in the diffusive-thermal model. The parameter, $\widetilde{q}$, denotes the reaction heat-release per unit mass of fuel. $\widetilde{A}$ is the pre-factor of Arrhenius law, $\widetilde{E}$ the activation energy, and $\widetilde{R}^0$ the universal gas constant.

The mixture-averaged diffusion model [10,17,25] is employed and the diffusive mass flux in Eq. (2) is

$$\widetilde{j}_Y=-\widetilde{\rho}\widetilde{D}\left(\frac{\partial \widetilde{Y}}{\partial \widetilde{r}}+\alpha\widetilde{Y}\frac{\partial \widetilde{T}}{\widetilde{T}\partial \widetilde{r}}\right) \tag{4}$$

in which the first term on the right hand side represents Fickian diffusion while the second term corresponds to Soret diffusion. $\widetilde{D}$ denotes the molecular diffusivity of fuel and α is the Soret coefficient which is negative for light species (hydrogen) and positive for heavy fuels (e.g. n-heptane, n-decane) [17,25].

Similar to our previous study [6], a constant energy flux, $\widetilde{Q}$, is locally deposited at the center to initialize the ignition kernel.

$$-\left(4\pi\widetilde{r}^2\widetilde{\lambda}\frac{\partial \widetilde{T}}{\partial \widetilde{r}}\right)_{\widetilde{r}\to 0}=\widetilde{Q} \tag{5}$$

This is a limitation of theoretical analysis since in practice the ignition energy deposition should be resolved in time and space. The employment of such a steady-state energy deposition is for the purpose to obtain analytical solution [6]. Nevertheless, as demonstrated by numerical simulation [6], this simplification does not prevent the model from predicting qualitatively correct results.

We introduce the following non-dimensional variables

$$t=\frac{\widetilde{t}}{\widetilde{\delta}_f^0/\widetilde{S}_u^0},\quad r=\frac{\widetilde{r}}{\widetilde{\delta}_f^0},\quad u=\frac{\widetilde{u}}{\widetilde{S}_u^0},\quad T=\frac{\widetilde{T}-\widetilde{T}_u}{\widetilde{T}_{ad}-\widetilde{T}_u},\quad Y=\frac{\widetilde{Y}}{\widetilde{Y}_u} \tag{6}$$

where $\widetilde{T}_u$ and $\widetilde{Y}_u$ denote the temperature and fuel mass fraction in the fresh mixture. The characteristic speed $\widetilde{S}_u^0$, characteristic length $\widetilde{\delta}_f^0=\widetilde{\lambda}/(\widetilde{\rho}\widetilde{C}_P\widetilde{S}_u^0)$, and characteristic temperature $\widetilde{T}_{ad}=\widetilde{T}_u+\widetilde{Y}_u\widetilde{q}/\widetilde{C}_P$ are, respectively, the laminar flame speed, flame thickness, and flame temperature of an adiabatic planar flame. We study spherical flame initiation and propagation in the coordinate attached to the moving flame front, $R = R(t)$. In this coordinate, $\xi = r - R(t)$, the flame can be considered as in a quasi-steady state (the validation of this quasi-steady assumption has been demonstrated by transient numerical simulation [6,8,9]) and thereby the non-dimensional governing equations become

$$-U\frac{dT}{d\xi}=\frac{1}{(\xi+R)^2}\frac{d}{d\xi}\left[(\xi+R)^2\frac{dT}{d\xi}\right]+\omega \tag{7}$$

$$-U\frac{dY}{d\xi}=\frac{Le^{-1}}{(\xi+R)^2}\frac{d}{d\xi}\left[(\xi+R)^2\left(\frac{dY}{d\xi}+\frac{\alpha Y}{\gamma+T}\cdot\frac{dT}{d\xi}\right)\right]-\omega \tag{8}$$

with

$$\omega=\frac{1}{2Le}\cdot Y\cdot Z^2\cdot\exp\left[\frac{Z(T-1)}{\sigma+(1-\sigma)T}\right] \tag{9}$$

where U is the non-dimensional flame propagation speed, $U = dR(t)/dt$, Le the Lewis numbers, $Le=\widetilde{\lambda}/(\widetilde{\rho}\widetilde{C}_P\widetilde{D})$, γ the temperature ratio, $\gamma=\widetilde{T}_u/(\widetilde{T}_{ad}-\widetilde{T}_u)$. Z is the Zel'dovich number, $Z=\widetilde{E}(1-\sigma)/\widetilde{R}^0\widetilde{T}_{ad}$ and σ the thermal expansion ratio, $\sigma=\widetilde{T}_u/\widetilde{T}_{ad}$.

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