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Effects of Soret Diffusion on Premixed Counterflow Flames

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Soret diffusion is a secondary mass diffusion and it affects laminar flames with very light or heavy species and large temperature gradients. To get a general understanding of Soret effects on stretched flames, we conduct theoretical analysis on a premixed counterflow flame with Soret diffusion. A deliberately idealized premixed counterflow flame model is analyzed asymptotically within the framework of large activation energy, potential flow, and thermal-diffusive model. A correlation among flame stretch rate, flame position, and flame temperature is derived and is used to assess the effects of Soret diffusion on counterflow flame structure, Markstein length, and extinction stretch rate. Results show that Soret diffusion quantitatively affects the premixed counterflow flame and that the influence of Soret diffusion strongly depends on Lewis number and stretch rate. For light fuels, the premixed counterflow flame becomes stronger after including Soret diffusion. The opposite trend occurs for heavy fuels. The influence of Soret diffusion is found to increase with the stretch rate. A linear change between normalized Markstein length and Soret diffusion coefficient is observed, indicating that flame becomes more sensitive to stretch rate after including Soret diffusion. Furthermore, Soret diffusion is shown to greatly increase the extinction stretch rate of light fuels. These results indicate that for highly-stretched premixed flames containing very light species, the impact of Soret diffusion cannot be neglected.

INTRODUCTION

Mass diffusion is extremely important in laminar flames since it drives reactants into a reaction zone in which chemical energy is converted into heat (Law, 2006). There are two main modes of mass diffusion in the combustion process: one is Fickian diffusion driven by concentration gradient and the other is Soret diffusion driven by temperature gradient (Hirschfelder et al., 1954). Fickian diffusion is the dominant mode of mass transport and it is always considered in laminar flame modeling. Compared to Fickian diffusion, Soret

diffusion is a secondary mass diffusion and it is only important for very light or very heavy species. In most studies on laminar flame structure and fundamental properties of laminar flames (e.g., laminar flame speed, extinction stretch rate, etc.), mass transport was merely represented by Fickian diffusion while little attention was paid to Soret diffusion. However, Soret diffusion is expected to be important for cases with sufficiently light or heavy species and strong temperature gradients (Hirschfelder et al., 1954).

In the literature, the effects of Soret diffusion have been mainly studied through numerical simulation. For examples, Rosner and coworkers (Gomez and Rosner, 1993; Rosner et al., 2000) investigated the Soret diffusion of heavy species, such as particle and soot; Ern and Giovangigli (1998, 1999) studied the influence of Soret diffusion on the extinction of hydrogen/air and methane/air flames; Xin et al. (2012) and Yang et al. (2010) found that extinction stretch rate can be greatly affected by Soret diffusion; and Bongers and de Goey (2003), Yang et al. (2010, 2011), and Liang et al. (2013) assessed the effects of the Soret diffusion on laminar flame speed. These numerical studies (Bongers and De Goey, 2003; Ern and Giovangigli, 1998, 1999; Gomez and Rosner, 1993; Liang et al., 2013; Rosner et al., 2000; Xin et al., 2012; Yang et al., 2010, 2011) indicated discernible effects of Soret diffusion in laminar flames containing very light or very heavy species. Unfortunately, numerical simulations are usually limited to specific fuel and, hence, the conclusions are lack of generality. To get a general understanding of Soret effects in combustion and to develop appropriate physical insight into the problem, analytical studies need to be conducted.

There are only a few theoretical studies on Soret effects in the literature. Garcia-Ybarra and colleagues (Garcia-Ybarra and Clavin, 1981; Garcia-Ybarra et al., 1984) considered Soret diffusion in their theoretical analysis and showed that thermo-diffusive stability limits and Markstein lengths are affected by Soret diffusion. Arias-Zugasti and Rosner (2008) assessed the influence of Soret diffusion on counterflow diffusion flames. They found that, besides the non-unity fuel Lewis number, the Soret diffusion induces additional shifts of flame temperature and position (Arias-Zugasti and Rosner, 2008). Fong et al. (2012) investigated the Soret diffusion effects on laminar diffusion flame residing in a counterflow of a fluid fuel stream and a gaseous oxidant. The flame temperature and position were found explicitly as a function of Soret diffusion coefficient (Fong et al., 2012). In these studies (Arias-Zugasti and Rosner, 2008; Fong et al., 2012; Garcia-Ybarra and Clavin, 1981; Garcia-Ybarra et al., 1984), the premixed counterflow flame was not considered. To our knowledge, in the literature there is no theoretical analysis on Soret diffusion effects on premixed counterflow flame.

Therefore, the present work aims to provide a general theoretical description of premixed counterflow flame with Soret diffusion and to assess the effects of Soret diffusion on counterflow flame structure, Markstein length, and extinction stretch rate. In the next section, theoretical model and analytical solutions are presented. Following that, the effects of Soret diffusion are examined. Finally, the conclusions are given in the last section.

THEORETICAL ANALYSIS

Mathematical Model

One-dimensional (1D), adiabatic, premixed counterflow flame is studied in the present theoretical analysis. Because of the symmetry in twin premixed counterflow flames, we only need to consider the half region of $0 \leq x < \infty$. Figure 1 shows the schematic
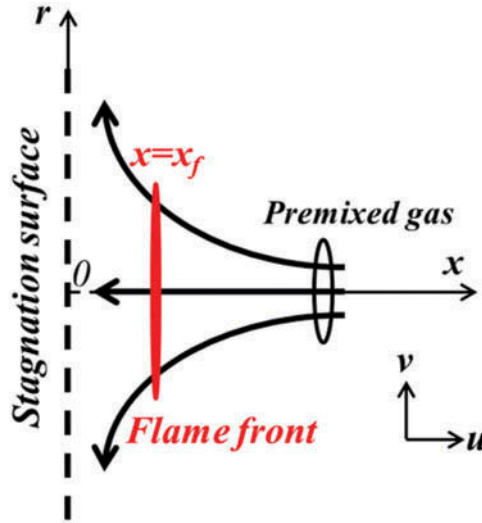
Figure 1 The schematic diagram of the premixed counterflow flame.

diagram of the premixed counterflow flame. For simplicity, we assume potential flow with velocity being $\tilde{u} = -\tilde{k}\tilde{x}$ and $\tilde{v} = \tilde{k}\tilde{r}/2$ (where $\tilde{k}$ is the stretch rate) without considering the boundary layer on the stagnation surface. A one-step, first-order, global reaction model is used and thereby the effects of radical (Zhang and Chen, 2011) and the coupling between Soret diffusion and chemical reaction (Liang et al., 2013) are not included in the present model. The mixture is assumed to be deficient in fuel and thus only fuel concentration needs to be considered. For the 1D, premixed, steady, counterflow flame, the governing equations for temperature $\tilde{T}$ and fuel mass fraction $\tilde{Y}$ are:

$$\tilde{\rho}\tilde{C}_P\tilde{u}\frac{d\tilde{T}}{d\tilde{x}} = \frac{d}{d\tilde{x}}\left(\tilde{\lambda}\frac{d\tilde{T}}{d\tilde{x}}\right) + \tilde{q}\tilde{\omega} \tag{1}$$

$$\tilde{\rho}\tilde{u}\frac{d\tilde{Y}}{d\tilde{x}} = -\frac{d}{d\tilde{x}}\left(\tilde{j}_Y\right) - \tilde{\omega} \tag{2}$$

For the sake of simplicity, we employ the diffusive-thermal model, according to which the density $\tilde{\rho}$, heat capacity $\tilde{C}_P$, and heat conductivity $\tilde{\lambda}$ of the mixture are all assumed to be constant. The parameter, $\tilde{q}$, in Eq. (1) denotes the reaction heat-release per unit mass of fuel. The reaction rate of the one-step global reaction is $\tilde{\omega} = \tilde{\rho}\tilde{A}\tilde{Y}\exp(-\tilde{E}/\tilde{R}^0\tilde{T})$, in which $\tilde{A}$ is the pre-factor of Arrhenius law, $\tilde{E}$ the activation energy, and $\tilde{R}^0$ the universal gas constant. The mixture-averaged diffusion model (Bongers and De Goey, 2003; Fong et al., 2012; Hirschfelder et al., 1954) is employed and the diffusive mass flux in Eq. (2) is:

$$\tilde{j}_Y = -\tilde{\rho}\tilde{D}\left(\frac{d\tilde{Y}}{d\tilde{x}} + \alpha\tilde{Y}\frac{d\tilde{T}}{\tilde{T}d\tilde{x}}\right) \tag{3}$$

in which the first term on the right-hand side represents mass flux due to Fickian diffusion while the second one is due to Soret diffusion. Here, $\tilde{D}$ denotes the molecular

diffusivity of fuel and α is the Soret diffusion coefficient. Since Soret diffusion drives light/heavy molecules towards a hot/cold region, the coefficient α is typically negative for light species (e.g., atomic and molecular hydrogen) and positive for heavy fuels (e.g., n-heptane, *n*-decane) (Bongers and De Goey, 2003; Fong et al., 2012; Hirschfelder et al., 1954).

The following nondimensional variables are introduced:

$$x = \frac{\tilde{x}}{\tilde{\delta}_f^0} \quad u = \frac{\tilde{u}}{\tilde{S}_L^0} \quad T = \frac{\tilde{T} - \tilde{T}_u}{\tilde{T}_{ad} - \tilde{T}_u} \quad Y = \frac{\tilde{Y}}{\tilde{Y}_u} \quad \omega = \frac{\tilde{\omega}\tilde{\delta}_f^0}{\tilde{\rho}\tilde{S}_L^0\tilde{Y}_u} \quad k = \tilde{k}\frac{\tilde{\delta}_f^0}{\tilde{S}_L^0} \tag{4}$$

where $\tilde{T}_u$ and $\tilde{Y}_u$ denote the temperature and fuel mass fraction in the fresh mixture. The characteristic speed $\tilde{S}_L^0$, characteristic length $\tilde{\delta}_f^0 = \tilde{\lambda}/(\tilde{\rho}\tilde{C}_P\tilde{S}_L^0)$, and characteristic temperature $\tilde{T}_{ad} = \tilde{T}_u + \tilde{Y}_u\tilde{q}/\tilde{C}_P$ are, respectively, the laminar flame speed, flame thickness, and flame temperature of an adiabatic, unstretched, planar flame. The nondimensional governing equations are:

$$\frac{d^2T}{dx^2} + kx\frac{dT}{dx} + \omega = 0 \tag{5}$$

$$\frac{d^2Y}{dx^2} + kLex\frac{dY}{dx} + \alpha\frac{d}{dx}(Yf) - \omega = 0 \tag{6}$$

in which $Le = \tilde{\lambda}/(\tilde{\rho}\tilde{C}_P\tilde{D})$ is the Lewis number of fuel. The boundary conditions are:

$$x = 0: \quad dT/dx = 0, \quad Y = 0 \tag{7}$$

$$x \to +\infty: \quad T = 0, \quad Y = 1 \tag{8}$$

In Eq. (6), f represents the so-called "driving force" of Soret diffusion (Yang et al., 2010; Yang et al., 2011):

$$f = \frac{1}{\tilde{T}}\frac{d\tilde{T}}{d\tilde{x}} = \frac{1}{\gamma + T}\frac{dT}{dx} \quad \text{with} \quad \gamma = \frac{\tilde{T}_\infty}{\tilde{T}_{ad} - \tilde{T}_\infty} \tag{9}$$

In the limit of large activation energy, chemical reaction occurs within a very thin zone of high temperature and the reaction rate can be replaced by the following Delta function (Joulin and Clavin, 1979; Veeraragavan and Cadou, 2011; Wu and Chen, 2012):

$$\omega = [\sigma + (1 - \sigma)T_f]^2 \exp\left[\frac{Z}{2}\frac{T_f - 1}{\sigma + (1 - \sigma)T_f}\right] \cdot \delta(x - x_f) \tag{10}$$

where $\sigma = \tilde{T}_u/\tilde{T}_{ad}$ is the thermal expansion ratio and $Z = \tilde{E}(1 - \sigma)/(\tilde{R}^0\tilde{T}_{ad})$ the Zel'dovich number.

By integrating Eq. (6) from the flame front to the fresh region, we have:

$$\left.\frac{dY}{dx}\right|_{x=x_f^+} = Le\int_{x_f^+}^{\infty}\left(kx\frac{dY}{dx}\right)dx \tag{11}$$

It is seen that the integration of the Soret term in Eq. (6) is equal to zero in the fresh region. However, this does not mean that the Soret effect does not affect the propagation of a strained premixed flat flame. It is noticed that there is an x before dY/dx in the convective term in Eq. (6). Therefore, the integration of this convection term is not a constant and it depends on the distribution of fuel mass fraction. After Soret diffusion of fuel is considered, the distribution of fuel mass fraction changes and so does the integration of the convection term in Eq. (6). Therefore, for a strained premixed flat flame, the integration of the convection term in Eq. (6) in the fresh region does depend on the value of the Soret diffusion coefficient. This is unlike the unstrained, 1D, premixed, planar flame, for which the integration of the convection term is equal to a constant and it does not depend on the value of Soret diffusion coefficient. Therefore, as shown in other numerical analysis (Xin et al., 2012; Yang et al., 2010), the stained premixed flat flame is affected by Soret diffusion.

Integrating Eqs. (5) and (6) around the flame interface $x = x_f$ yields the following jump relations:

$$\left.\frac{dT}{dx}\right|_{x_f^-} - \left.\frac{dT}{dx}\right|_{x_f^+} = \frac{1}{Le}\left(\left.\frac{dY}{dx}\right|_{x_f^+} - \left.\frac{dY}{dx}\right|_{x_f^-}\right) = [\sigma + (1-\sigma)T_f]^2 \exp\left[\frac{Z}{2}\frac{T_f - 1}{\sigma + (1-\sigma)T_f}\right] \tag{12}$$

Analytical Solution

Without the nonlinear reaction term, Eqs. (5) and (6) subjected to conditions given by Eqs. (7), (8), and (12) can be solved analytically in the unburned ($x \geq x_f$) and burned ($0 \leq r \leq x_f$) zones. The analytical solution for the temperature distribution is:

$$T(x) = \begin{cases} T_f & \text{for } 0 \leq x \leq x_f \\ T_f I(x,k)/I(x_f,k) & \text{for } x \geq x_f \end{cases} \tag{13}$$

where $I(x,k) = \int_x^\infty \exp(-ks^2/2)ds$ and T_f is the flame temperature to be determined later.

For fuel-lean case, fuel is completely consumed in a flame front and it appears only in the unburned zone. It is noted that we always have $f < 0$ since the temperature gradient is always negative in the unburned zone (see Eqs. (13) and (9)). Since Soret diffusion is usually one order smaller than Fickian diffusion, Eq. (6) can be solved asymptotically. By neglecting the second and higher-order terms of $O(\alpha^2)$, we obtain the following expression for fuel mass fraction in the unburned zone ($x \geq x_f$):

$$Y(x) = Y_0(x) + \alpha Y_1(x) \tag{14}$$

$$Y_0(x) = 1 - I(x,kLe)/I(x_f,kLe) \tag{15}$$

$$Y_1(x) = 1 - \frac{I(x,kLe)}{I(x_f,kLe)}\int_{x_f}^\infty \frac{F(s)Y_0(s)}{dY_0(s)/ds}ds + \int_x^\infty \frac{F(s)[Y_0(s) - Y_0(x)]}{dY_0(s)/ds}ds \tag{16}$$

where $F(x) = -d(Y_0 f)/dx$ and $f(x)$ is defined in Eq. (9).

Substituting Eqs. (13)–(16) into the jump relations in Eq. (12), we obtain the following algebraic system of equations for stretch rate, k, flame position, x_f, and flame temperature, T_f:

$$T_f \frac{e^{-kx_f^2/2}}{\int_{x_f}^{\infty} e^{-k\xi^2/2}d\xi} = \frac{1}{Le} \frac{e^{-kLex_f^2/2}}{\int_{x_f}^{\infty} e^{-kLe\xi^2/2}d\xi} \left[1 + \alpha \int_{x_f}^{\infty} G(\xi)d\xi\right]$$
$$= [\sigma + (1-\sigma)T_f]^2 \exp\left[\frac{Z}{2} \frac{T_f - 1}{\sigma + (1-\sigma)T_f}\right] \tag{17}$$

in which

$$G(x) = T_f \frac{I(x, kLe)}{I(x_f, kLe)}$$

$$\times \left\{\frac{kx \cdot e^{k(Le-1)x^2/2}[I(x_f, kLe) - I(x, kLe)] - e^{-kx^2/2}}{\gamma I(x_f, k) + T_f I(x, k)} - \frac{T_f e^{k(Le-2)x^2/2}[I(x_f, kLe) - I(x, kLe)]}{[\gamma I(x_f, k) + T_f I(x, k)]^2}\right\} \tag{18}$$

By numerically solving Eq. (17) using the Newton's iteration method, we can get the flame position (x_f), flame speed ($S_L = kx_f$), and flame temperature (T_f) as a function of flame stretch (k) for different Lewis numbers (Le) and Soret diffusion coefficients (α). When the Soret diffusion is neglected (i.e., $\alpha = 0$), Eq. (17) reduces to:

$$T_f \frac{e^{-kx_f^2/2}}{\int_{x_f}^{\infty} e^{-k\xi^2/2}d\xi} = \frac{1}{Le} \frac{e^{-kLex_f^2/2}}{\int_{x_f}^{\infty} e^{-kLe\xi^2/2}d\xi} = \left[\sigma + (1-\sigma)T_f\right]^2 \exp\left[\frac{Z}{2} \cdot \frac{T_f - 1}{\sigma + (1-\sigma)T_f}\right] \tag{19}$$

which is the same as the previous results on adiabatic premixed counterflow flame (Chen and Ju, 2008; Ju et al., 2000). Therefore, in the limit of $\alpha = 0$ the present analysis is consistent with previous studies without considering Soret diffusion.

It is noted that the deliberately idealized theoretical analysis is constrained by the assumptions of one-step chemistry, large activation energy, constant thermal and transport properties, and potential flow field. Other factors, such as thermal expansion, boundary layer on the stagnation surface, and temperature-dependent diffusivities, are not taken into consideration. Therefore, the present theoretical analysis only provides qualitative information on the influence of Soret diffusion on premixed counterflow flame.

RESULTS AND DISCUSSION

In the present study, emphasis is placed on examining the Soret diffusion effects on stretched flame speed, Markstein length, extinction stretch rate, and flame structure of premixed counterflow flame. Results at different values of Soret diffusion coefficient and Lewis number are obtained from Eq. (17). The Zel'dovich number, $Z = 10$, and thermal expansion ratio, $\sigma = 0.22$ and $\gamma = \sigma/(1-\sigma) = 0.282$, are fixed. We consider two Lewis numbers, $Le = 0.5$ and $Le = 2.0$, which represent light and heavy fuels, respectively. Since the Soret diffusion coefficient, α, is negative/positive for light/heavy species, we have $\alpha = -0.1$ for $Le = 0.5$ and $\alpha = +0.1$ for $Le = 2.0$. The approximate value of Soret diffusion coefficient is $\alpha = -0.29$ for hydrogen molecule at high temperature (Fristrom and

Monchick, 1988) and its absolute value decreases for hydrogen in the low-temperature pre-heat zone. As mentioned before, the Soret diffusion coefficient is assumed to be a constant, which is a limitation of the present analysis. Therefore, we choose an approximately averaged value of $\alpha = -0.1$ for light fuels. It is noted that the value of α is somewhat arbitrarily chosen. Nevertheless, the same conclusion can be drawn even when other values of α are used since the theory works for all different values of α.

Figure 2a shows the change of flame position, x_f, with the stretch rate, k. It is observed that the flame approaches to the stagnation surface as the stretch rate increases. For both cases, there is a critical value of the stretch rate, beyond which the flame cannot exist. The critical stretch rate is the so-called extinction stretch rate and it is denoted by K_{ext}. For $Le = 0.5$, flame extinction occurs when the flame is close to the stagnation surface. However, for $Le = 2.0$, flame extinction occurs at the turning point on the x_f-k curve. The completely different extinction behavior for different Lewis numbers is due to the coupling between positive stretch rate and non-unity Lewis number (preferential diffusion between fuel and heat). The readers are referred to Law (2006) for a detailed explanation.

Figures 2b and 2c show the influence of Soret diffusion on stretched flame speed, S_L, and flame temperature, T_f. The flame temperature is slightly affected by Soret diffusion and the influence becomes stronger as the extinction stretch rate is approached. Since the flame speed depends on flame temperature in the Arrhenius form with large activation energy, the stretched flame speed is shown to be much more strongly affected by Soret diffusion than flame temperature.

For light fuel with $Le = 0.5$, Figure 2 shows that flame position, stretched flame speed, and flame temperature become larger after considering Soret diffusion (i.e., the Soret diffusion coefficient changes from $\alpha = 0$ to $\alpha = -0.1$). This indicates that the premixed counterflow flame becomes stronger and more difficult to be extinguished after including Soret diffusion. This is reasonable since Soret diffusion facilitates mass transport of light fuel towards the high-temperature reaction zone (see Figure 3) and thereby leads to approaching stoichiometry for the lean flame and increase of the burning intensity. On the other hand, for heavy fuel with $Le = 2.0$, Figure 2 indicates that the premixed counterflow flame becomes weaker after considering Soret diffusion (α changes from $\alpha = 0$ to $\alpha = +0.1$). This is because Soret diffusion inhibits mass transport of heave fuel towards the reaction zone (see Figure 3) and thereby leads to further departure from stoichiometry. The theoretical results shown in Figure 2 are compatible with those from simulation considering detailed chemistry and transport (Xin et al., 2012; Yang et al., 2010): for premixed counterflow flame of lean H_2/air (the equivalence ratio is $\phi = 0.35$), numerical simulation by Yang et al. (2010) showed that the flame becomes stronger after considering the Soret diffusion of hydrogen molecule; and for lean nC_7H_{16}/air ($\phi = 0.6$), numerical simulation by Xin et al. (2012) showed that the flame becomes weaker after considering the Soret diffusion of heptane molecule.

In order to interpret the dependence of Soret diffusion influence on stretch rate, we examine the fuel transport to reaction zone due to Fickian diffusion and that due to Soret diffusion. These two mass fluxes are calculated according to the following expressions:

$$J_{\text{Fickian}} = \frac{1}{Le} \left.\frac{dY_0(x)}{dx}\right|_{x=x_f} \qquad J_{\text{Soret}} = \frac{\alpha}{Le} \left.\frac{dY_1(x)}{dx}\right|_{x=x_f} \qquad (20)$$

where $Y_0(x)$ and $Y_1(x)$ are, respectively, given in Eqs. (15) and (16). Figure 3 shows the ratio between J_{Soret} and J_{Fickian} as a function of stretch rate for $Le = 0.5$ and $Le = 2$.
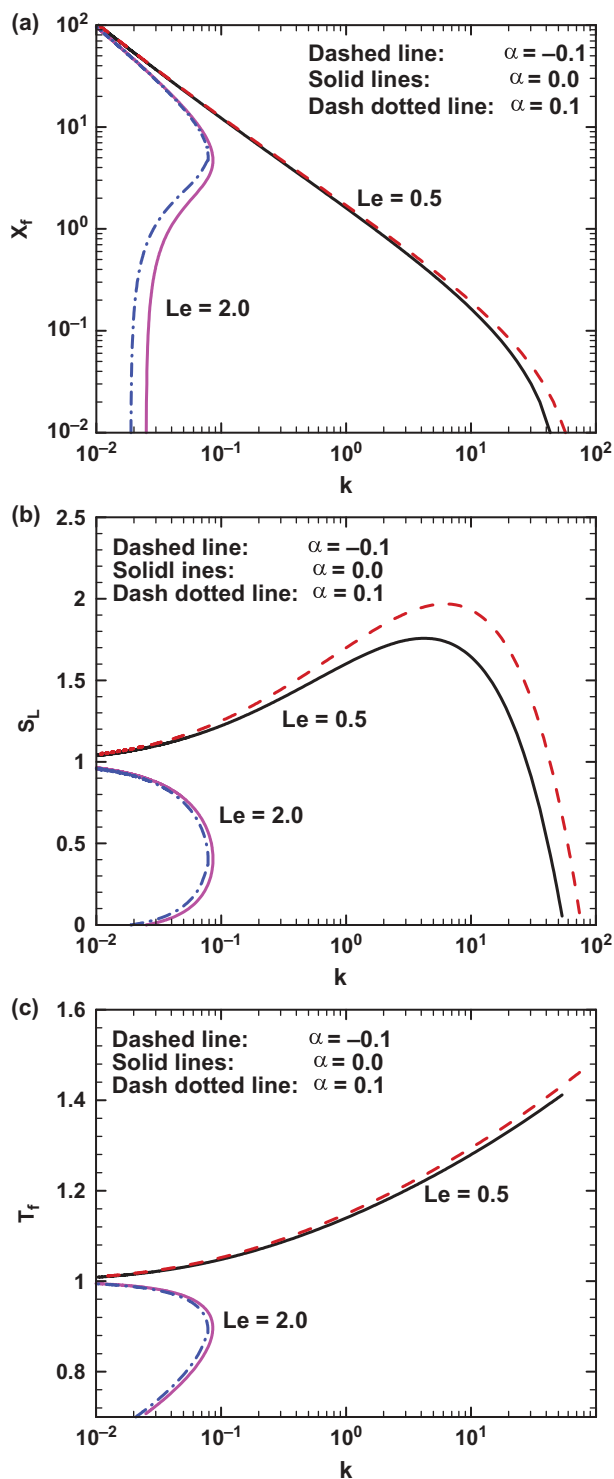
Figure 2 Change of the (a) flame position, (b) stretched flame speed, and (c) flame temperature with the stretch rate for light (*Le* = 0.5) and heavy fuel (*Le* = 2.0).
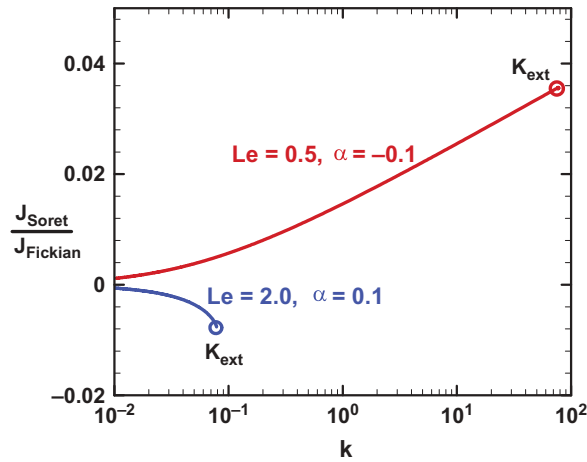
Figure 3 The ratio between fuel transportation to the reaction zone due to Soret diffusion, J_{Soret}, and that due to Fickian diffusion flux, J_{Fickian}, as a function of stretch rate for $Le = 0.5$ and $Le = 2.0$.

As expected, the mass flux due to Soret diffusion is much smaller than that due to Fickian diffusion. It is observed from Figure 3 that the Soret effect on the net diffusive flux is merely a few percent, which is due to the factor Y/T in the Soret diffusion term (see Eq. (3))—as the mixture approaches the reaction zone, Y decreases and T increases. For light fuel with $Le = 0.5$ and $\alpha = -0.1$, both J_{Soret} and J_{Fickian} are positive, indicating that Soret diffusion increases the equivalent mass diffusivity and thereby reduces the effective Lewis number. For heavy fuel with $Le = 2.0$ and $\alpha = +0.1$, we have $J_{\mathrm{Soret}} < 0 < J_{\mathrm{Fickian}}$, indicating that Soret diffusion reduces the equivalent mass diffusivity and thereby increases the effective Lewis number. It is well known that positively stretched flame becomes stronger/weaker at smaller/larger Lewis number (Law, 2006). Therefore, Soret diffusion strengthens and weakens the premixed counterflow flame for $Le = 0.5$ and $Le = 2.0$, respectively.

Figure 3 also shows that the ratio, $|J_{\mathrm{Soret}}/J_{\mathrm{Fickian}}|$, increases with the stretch rate, indicating that Soret diffusion has a stronger influence at a higher stretch rate. This is consistent with results in Figure 2. With the increase of stretch, the flame front moves toward the stagnation surface (see Figure 2a) and the preheat zone becomes narrower. Consequently, the temperature gradient and thereby Soret diffusion increase with stretch rate. This is demonstrated by Figure 4, which shows the temperature and fuel mass fraction distributions at different stretch rates for $Le = 0.5$. At a fixed stretch rate, Soret diffusion is shown to modify the distributions of temperature and fuel mass fraction and promotes the fuel transport to the reaction zone. When the stretch rate is increased from 0.1 K_{ext} to 0.9 K_{ext}, the flame becomes closer to the stagnation surface and both temperature and fuel mass fraction gradients are shown to increase.

The Markstein length/number is used to characterize the influence of external stretching on local flame speed. For weakly stretched flames, there is a linear relationship between the stretched flame speed, S_L, and stretch rate, k (i.e., $S_L = S_L^0 - L \cdot k$, where S_L^0 is the flame speed at zero stretch rate). Therefore, Markstein length, L, can be obtained from linear extrapolation between S_L and k. The Markstein length at different Soret diffusion coefficients are obtained and the normalized results for $Le = 0.5$ and $Le = 2.0$ are shown in Figure 5. It is seen that the normalized Markstein length increases linearly with the absolute

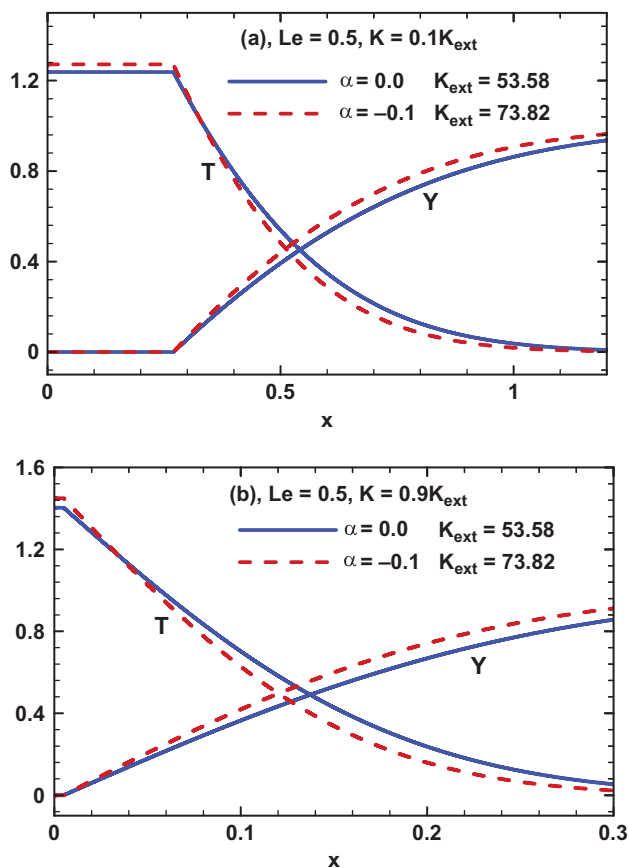**Figure 4** Temperature and fuel mass fraction distributions with and without considering Soret diffusion.
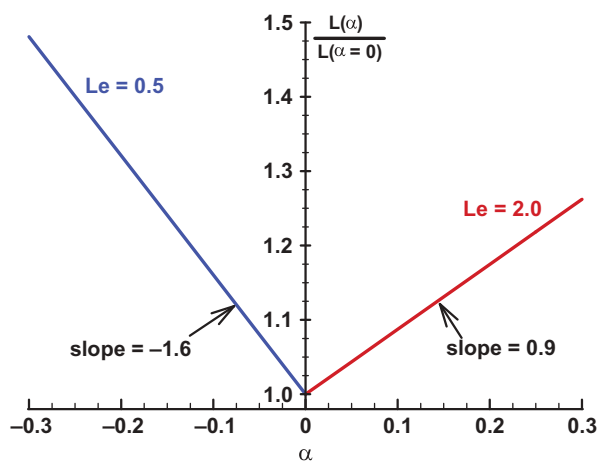

Figure 5 Markstein length L as a function of Soret diffusion coefficient for $Le = 0.5$ and $Le = 2.0$.

value of Soret diffusion coefficient. This indicates that for both light and heavy fuels, the stretched flame speed becomes more sensitive to stretch rate after including Soret diffusion. This observation is also consistent with the previous discussion on the change of effective Lewis number by Soret diffusion. After including Soret diffusion, the effective Lewis number decreases/increases for $Le = 0.5/Le = 2.0$ and thereby the stretch effects become stronger. Furthermore, it is observed that the influence of Soret diffusion on Markstein length of light fuel with $Le = 0.5$ is much stronger that on Markstein length of heavy fuel with $Le = 2.0$. This is due to the fact that the higher flame temperature and temperature gradient at smaller Lewis number induces stronger Soret diffusion.

Besides the Markstein length, the influence of Soret diffusion on the extinction stretch rate is also studied. It is noted that the extinction strain rate is highly sensitive to the variations in the diffusive properties. The presence of Soret diffusion can decrease/increase the effective Lewis numbers of light/heavy fuels (Han and Chen, 2015). Therefore, it is expected that Soret diffusion can have a relatively strong influence on the extinction strain rate for flames containing sufficiently light/heavy fuels. Figure 6 shows the normalized extinction stretch rate as a function of Soret diffusion coefficient for light fuel with $Le = 0.5$ and heavy fuel with $Le = 2.0$. Consistent with results in Figure 2, Soret diffusion increases and decreases the extinction stretch rate for light fuel ($Le = 0.5$) and heavy fuel ($Le = 2.0$), respectively. Specifically, the extinction stretch rate is increased by 38% for light fuel with $Le = 0.5$ after α is changed from 0 to -0.1 and it is reduced by 8.7% for heavy fuel with $Le = 2.0$ after α is changed from 0 to $+0.1$. Therefore, Soret diffusion should be considered when the extinction stretch rate is used in chemical mechanism validation and development. In fact, simulation with detailed chemistry (Xin et al., 2012; Yang et al., 2010) also indicated discernible effects of Soret diffusion on the extinction stretch rate: for premixed counterflow flame of lean H_2/air (the equivalence ratio is $\phi = 0.35$), Yang et al. (2010) showed that extinction stretch rate is increased by 24% after considering the Soret diffusion of hydrogen molecule; and for lean nC_7H_{16}/air ($\phi = 0.6$), Xin et al. (2012) showed that the extinction stretch rate is reduced by 18% after considering the Soret diffusion of heptane molecule. Moreover, Figure 6 indicates that the
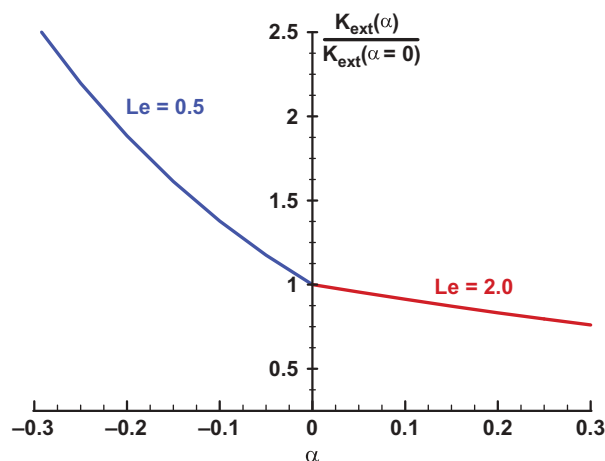

Figure 6 The normalized extinction stretch rate as a function of Soret diffusion coefficient for $Le = 0.5$ and $Le = 2.0$.

sensitivity of extinction stretch rate of light fuel to Soret diffusion is much stronger than that of heavy fuel. Therefore, Soret diffusion has a strong influence on the extinction of lean premixed counterflow flames containing very light species, such as atomic and molecular hydrogen.

CONCLUSIONS

A simplified premixed counterflow flame model including Soret diffusion is analyzed within the framework of large activation energy and potential flow. A general correlation among flame stretch rate, flame position, and flame temperature is derived. It is used to assess the Soret diffusion effects on premixed counterflow flame structure, Markstein length, and extinction stretch rate at different Lewis numbers. It is found that Soret diffusion quantitatively affects the flame position, flame temperature, and stretched flame speed of premixed counterflow flame and that the influence of Soret diffusion greatly depends on Lewis number and stretch rate. For light fuel with $Le < 1$, the premixed counterflow flame becomes stronger and more difficult to be extinguished after including Soret diffusion. The opposite trend occurs for heavy fuel with $Le > 1$. This is due to the fact that Soret diffusion facilitates/inhabits mass transport of light/heavy fuel towards the reaction zone and thus modifies the local stoichiometry. With the increase of stretch rate, the mass transport due to Soret diffusion increases and thereby Soret diffusion has a stronger influence at higher stretch rate. Furthermore, it is shown that the normalized Markstein length linearly increases with the Soret diffusion coefficients, indicating that for both light and heavy fuels, the stretched flame speed becomes more sensitive to stretch rate after including Soret diffusion. In terms of extinction stretch rate, it is increased by Soret diffusion for light fuel. Therefore, for the extinction of lean premixed counterflow flames containing very light species, the Soret diffusion effects should be considered.

It is noted that near-limit combustion processes, such as extinction and ignition, are much more sensitive to Soret diffusion than the normal flame propagation process. Besides, the Soret diffusion is important for cases with sufficiently light or heavy species and strong temperature gradients and it can be negligible for normal hydrocarbon fuels. As suggested by one of the anonymous reviewers, the uncertainties in diffusive coefficients in the case of detailed flame calculations might be much larger than the Soret diffusion coefficient, which is difficult to accurately estimate. Therefore, the importance of the Soret diffusion effect should not be overemphasized.

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