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Asymptotic Analysis of Radiative Extinction in Counterflow Diffusion Flames of Nonunity Lewis Numbers

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The effects of radiation heat loss and variation in near-unity Lewis numbers on the structure and extinction of counterflow diffusion flame established near the stagnation plane of two opposed free streams of fuel and oxidizer are analyzed using the asymptotic method of large activation energy. Radiation heat loss from the reaction zone is accounted for using the optically thin assumption. The main concern of this study is the thermal effects of radiation heat loss and Lewis numbers on diffusion flame extinction, particularly at small stretch rates. The existence of two extinction limits, the radiation extinction limit at a small stretch rate and the conventional quenching limit at a large stretch rate, is theoretically reproduced. This simplified analysis is able to predict the existence of inflammable limits of counterflow diffusion flames in terms of the near-unity Lewis numbers and concentrations of the fuel and oxidizer streams. Crown copyright © 2000. Published by Elsevier Science Inc. All rights reserved.

NOMENCLATURE

a	stretch rate
A	constant defined in Eq. 50
B	preexponential factor
c	heat loss parameter defined in Eq. 66
c_p	specific heat
D	mass diffusion coefficient
Da	Damköhler number
k	configuration factor
K_p	Planck mean absorption coefficient
Le	Lewis number
m	heat loss parameter defined in Eq. 51
q_r	heat loss term due to radiation
Q	heat of combustion
T	temperature
T_a	nondimensional activation energy
W	molecular weight
y	mass fraction perturbation in the reaction zone
Y	mass fraction
z	transformed coordinate defined in Eq. 15

ρ	density
γ	stoichiometric oxidizer to fuel mass ratio
σ	Stefan-Boltzmann constant
ϵ	small parameter, defined as T_f^2/T_a
ϵ_r	small parameter defined in Eq. 17
θ	temperature perturbation in the reaction zone
θ_r	temperature perturbation in the radiation zone
ξ	stretched coordinate defined in Eq. 43
ξ_r	inner coordinate defined in Eq. 20
ω	nondimensional reaction rate defined in Eq. 4
Ψ	transformed variable defined in Eq. 60
ψ	transformed variable defined in Eq. 61
Λ	reduced Damköhler number

Subscripts

F	fuel
O	oxidizer
e	extinction
f	flame

Greek Symbols

η	nondimensional axial coordinate
λ	heat conduction coefficient

INTRODUCTION

Extinction of diffusion flames due to a short residence time at high stretch has been exten-

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sively analyzed using the asymptotic method of large activation energy [1–3]. Flame extinction can be primarily attributed to excessive heat loss from the reaction zone. This is perhaps the physical reason behind the success of using a one-step irreversible reaction in almost all the theoretical and some numerical studies. Heat loss from the reaction zone is through the mechanisms of both conduction and radiation. Their relative importance can be quite different under different conditions, including flame size, flame stretch, and Lewis numbers.

Although the potential importance of radiation heat loss on flame extinction was pointed out by Bonne in 1971 [4], it did not receive adequate research attention until the 1980s. An extensive review of radiative extinction of diffusion flame has recently been presented by T'ien and Bedir [5]. The first asymptotic analysis of the effect of radiation heat loss from the reaction zone on diffusion flame was perhaps conducted by Sohrab et al. [6]. In their work, the extinction condition of diffusion flame in a stagnation-point boundary layer subject to radiation heat loss from the flame was obtained. While the reduction of flame temperature by radiation heat loss was demonstrated, the existence of radiation extinction at a low stretch rate was not realized. Using a one-step irreversible reaction and constant transport properties, T'ien [7] first numerically demonstrated the existence of an upper and a lower extinction stretch rate for the steady burning of a counterflow diffusion flame in the stagnation point region of a condensed fuel with radiative heat loss from the fuel surface. He also showed that there exists a flammability limit in terms of the oxygen concentration. The radiation heat loss from the reaction zone, however, was not considered. In their numerical study of a laminar $\text{CO-H}_2\text{-N}_2/\text{air}$ diffusion flame stabilized near the stagnation point of the Tsuji flow configuration using detailed chemistry and transport properties, Liu and Rogg [8] showed that the flame temperature continues to decrease with decreasing the stretch rate when radiation heat loss from the flame is considered. They suggested the existence of a radiation extinction limit at low stretch. Chao et al. [9] were the first to demonstrate the existence of radiation extinction of diffusion flame in their study of

effects of flame radiation heat loss from droplet diffusion flame using the asymptotic analysis. By solving numerically the diffusion flamelet governing equations formulated in the mixture fraction space with radiation heat loss using the optically thin assumption and the skeletal mechanism for methane–air combustion, Liu et al. [10] found that the flame temperature decreases as the scalar dissipation rate decreases and flame extinction occurs at a sufficiently small dissipation rate. More recently, extinction of low-stretched counterflow diffusion flame in microgravity has been investigated both experimentally and numerically by Maruta et al. [11]. Their study confirms the existence of radiation extinction at low stretch. In addition, they obtained the flammability limit of the counterflow diffusion flame in terms of the fuel concentration.

More recent theoretical studies using the asymptotic method of large activation energy on the extinction of diffusion flames due to radiation heat loss have been conducted by Chao and Law [12], Oh et al. [13], and Mills and Matalon [14]. Most of the theoretical studies make the assumption of unity Lewis numbers with only a few exceptions such as the studies by Chung and Law [3] and Mills and Matalon [14]. Mills and Matalon showed that the Lewis numbers have a significant effect on the structure and extinction of spherical diffusion flame and when the Lewis numbers are sufficiently high steady burning becomes impossible. On the other hand, recent numerical and analytical examinations of the Lewis number effect on the radiative premixed flame showed that the variance of Lewis number greatly enriches the phenomena and yields various flame regimes and bifurcations [15–18].

Understanding of the combined effect of Lewis number and radiation on the structure and extinction of laminar diffusion flame established near the stagnation plane of two opposed free streams of fuel and oxidizer is of particular importance for the application of the laminar flamelet model to turbulent nonpremixed combustion since it is under this flame configuration that the flamelet library is calculated. This work is motivated by the importance of this flame and the fact that the effects of radiation heat loss and nonunity Lewis numbers on such flame may have not been analyzed from a theoretical point of view.

In the present study, the effects of radiation heat loss from the reaction zone and nonunity Lewis numbers of fuel and oxidizer on the structure and extinction of counterflow diffusion flame formed near the stagnation plane of two opposed free streams were analyzed using the asymptotic method of large activation energy. The emphasis of this study is on the thermal consequence of radiation heat loss on the flame temperature.

ANALYSIS

The axisymmetrical counterflow configuration is considered in this study. A diffusion flame is established near the stagnation point of two counterflow streams of fuel and oxidizer with the fuel stream approaching the flame from the left-hand side ($-\infty$) and the oxidizer stream from the right-hand side (∞). Assuming constant physical and chemical properties of fuel and oxidizer streams, incompressible fluid, and equal free-stream velocities, governing equations can be written as [1, 3]

$$\frac{d^2T}{d\eta^2} + \eta \frac{dT}{d\eta} = \omega + q_r \quad (1)$$

$$\frac{1}{Le_F} \frac{d^2Y_F}{d\eta^2} + \eta \frac{dY_F}{d\eta} = -\omega \quad (2)$$

$$\frac{1}{Le_O} \frac{d^2Y_O}{d\eta^2} + \eta \frac{dY_O}{d\eta} = -\omega \quad (3)$$

where

$$\omega = -D_a Y_O Y_F \exp(-T_a/T) \quad (4)$$

is the nondimensional reaction rate of the one-step second-order irreversible reaction assumed in the present study and the Damköhler number is given as

$$D_a = \frac{\bar{\rho} \bar{B} \gamma}{\bar{W}_F k \bar{a}} \quad (5)$$

In this study, variables with and without overbar denote dimensional and nondimensional quantities, respectively. In the above equations, $\bar{\rho}$ is density, $\bar{B}$ is the preexponential factor, $\bar{Y}_{F,-\infty}$ the fuel mass fraction in the fuel stream, $\bar{W}_F$ the molecular weight of fuel, k the configuration factor (1 for planar geometry and 2 for axisym-

metrical case), $\bar{a}$ the stagnation-point velocity gradient or the stretch rate. Temperature is normalized by $\bar{Q}/\bar{c}_p$ with $\bar{Q}$ and $\bar{c}_p$ denoting the heat of combustion per unit mass of fuel and the specific heat at constant pressure respectively. Fuel and oxygen mass fractions are normalized by 1 and γ , respectively, with γ being the stoichiometric oxidizer to fuel mass ratio. In the reaction rate equation, T_a is the nondimensional activation energy. The axial coordinate η is normalized by $\sqrt{\bar{\lambda}/\bar{\rho} \bar{c}_p \bar{a} k}$ and Le_F and Le_O are the Lewis numbers of fuel and oxidizer streams, respectively. The Lewis number is defined as $\bar{\lambda}/(\bar{c}_p \bar{\rho} \bar{D})$ with $\bar{\lambda}$ and $\bar{D}$ denoting the heat and mass diffusion coefficients, respectively. Although density can be related to temperature through the ideal gas law, in the present analysis density is treated as constant for simplicity. This simplified treatment of density does not qualitatively affect the results of the analysis.

The radiation sink term in Eq. 1 is made nondimensional by $\bar{\rho} \bar{Q} \bar{a} k$. Using the optically thin approximation and assuming the ambient temperature is low, the nondimensional radiation heat loss term is given as

$$q_r = \frac{4\bar{K}_p \sigma \bar{Q}^3 T^4}{\bar{c}_p^4 \bar{\rho} \bar{a} k} \quad (6)$$

where $\bar{K}_p$ and σ are the Planck mean absorption coefficient and the Stefan-Boltzmann constant.

The boundary conditions are

$$\begin{aligned} \eta \rightarrow -\infty: \quad T &= T_{-\infty}, \\ Y_F &= \bar{Y}_{F,-\infty}, \\ Y_O &= 0 \\ \eta \rightarrow \infty: \quad T &= T_{\infty}, \quad Y_F = 0, \quad Y_O = \bar{Y}_{O,\infty}/\gamma \end{aligned} \quad (7)$$

In the limit of large activation energy, chemical reaction is confined to a very thin region of thickness of $O(\epsilon)$ called the reaction zone. The small parameter ϵ is defined as T_f^2/T_a and T_f is the flame temperature. Since radiation heat loss depends on the Planck mean absorption coefficient and strongly on temperature, it is important only in a small region around the reaction zone where the gas temperature and the concentrations of radiating species (namely soot,

Fig. 1. Schematic of the three-zone analysis of the counter-flow diffusion flame.

CO_2 , and H_2O) are high. In view of this analysis, the problem of interest can be divided into three regions: the inner reaction zone of thickness of $O(\epsilon)$, the radiation-convection-diffusion zone of thickness of $O(\epsilon_r)$ (ϵ_r will be defined later), and the outer convection-diffusion zone. Figure 1 illustrates these three zones. The radiation-convection-diffusion zone is assumed to be much thinner than that of the outer convection-diffusion zone, but is much thicker than the inner reaction zone which is sandwiched.

In this work, it is also assumed that the radiation heat loss is of $O(\epsilon)$ of the chemical heat release and the Lewis numbers of fuel and oxidizer streams are allowed to deviate from unity only by $O(\epsilon)$ in order to simplify the analysis.

Outer Convection-Diffusion Zone

In the outer convection-diffusion zone, chemical reaction and radiation heat loss can be neglected to the leading order. Solutions of temperature and mass fractions of fuel and oxidizer can be obtained by integrating Eqs. 1–3 along with the boundary conditions given in Eqs. 7 and 8. At $\eta < \eta_f$,

$$T = T_{-\infty} + \frac{T_f - T_{-\infty}}{\int_{-\infty}^{\eta_f} \exp\left(-\frac{1}{2}t^2\right) dt} \int_{-\infty}^{\eta} \exp\left(-\frac{1}{2}t^2\right) dt \quad (9)$$

$$Y_F = Y_{F,-\infty} - \frac{Y_{F,-\infty}}{\int_{-\infty}^{\eta_f} \exp\left(-Le_F \frac{1}{2}t^2\right) dt} \int_{-\infty}^{\eta} \exp\left(-Le_F \frac{1}{2}t^2\right) dt \quad (10)$$

$$Y_O = 0 \quad (11)$$

At $\eta > \eta_f$,

$$T = T_{\infty} + \frac{T_f - T_{\infty}}{\int_{\eta_f}^{\infty} \exp\left(-\frac{1}{2}t^2\right) dt} \int_{\eta}^{\infty} \exp\left(-\frac{1}{2}t^2\right) dt \quad (12)$$

$$Y_F = 0 \quad (13)$$

$$Y_O = Y_{O,\infty} - \frac{Y_{O,\infty}}{\int_{\eta_f}^{\infty} \exp\left(-Le_O \frac{1}{2}t^2\right) dt} \int_{\eta}^{\infty} \exp\left(-Le_O \frac{1}{2}t^2\right) dt \quad (14)$$

The outer solutions given in Eqs. 9–14 are those in the flame sheet limit. Expansion terms appear when finite rate kinetics is considered. In the limit of large activation energy, the role of radiation heat loss is to reduce the flame temperature in a narrow region (narrow relative to the outer convection-diffusion zone of the problem but still much thicker than the flame thickness, Fig. 1) around the reaction zone but not to change the mass fractions of fuel and oxidizer to the leading order.

Radiation-Convection-Diffusion Zone

In the intermediate radiation-convection-diffusion zone, chemical reaction can still be neglected. By using a transformed coordinate z defined as

$$z = \int_{-\infty}^{\eta} \exp\left(-\frac{1}{2}t^2\right) dt \quad (15)$$

the energy equation, Eq. 1, can now be written as

$$\frac{d^2 T}{dz^2} = q_r \exp(\eta^2) \quad (16)$$

Following the analysis of Sohrab et al. [6], the thickness of the radiation-convection-diffusion zone can be considered as $O(\epsilon_r)$ with

$$1 \gg \epsilon_r = \frac{d \ln T}{d \ln q_r} \gg \epsilon \quad (17)$$

With the constant density and constant properties assumptions made in this study, $\epsilon_r = 0.25$ based on Eq. 6. It has been shown by Sohrab et al. [6] that the radiation heat loss term and the temperature can be approximated in terms of ϵ_r as

$$q_r = q_{rf} \exp\left(\frac{T - T_f}{\epsilon_r T_f}\right) \quad (18)$$

$$T = T_f + \epsilon_r \theta_r \quad (19)$$

where q_{rf} is the radiation heat loss term at the flame location and θ_r denotes the deviation of temperature from the flame temperature.

Using an inner coordinate defined as

$$\xi_r = \frac{z - z_f}{\epsilon_r} \quad (20)$$

the energy equation, Eq. 16, can now be written as

$$\frac{d^2 \theta_r}{d \xi_r^2} = \epsilon_r q_{rf} \exp\left(\eta_f^2 + \frac{\theta_r}{T_f}\right) \quad (21)$$

Using the following relationship

$$\frac{d}{d \xi_r} \left[\left(\frac{d \theta_r}{d \xi_r} \right)^2 \right] = 2 \frac{d \theta_r}{d \xi_r} \frac{d^2 \theta_r}{d \xi_r^2} \quad (22)$$

and Eq. 21, one obtains

$$\frac{d}{d \xi_r} \left[\left(\frac{d \theta_r}{d \xi_r} \right)^2 \right] = 2 \epsilon_r q_{rf} \exp(\eta_f^2) \exp\left(\frac{\theta_r}{T_f}\right) \frac{d \theta_r}{d \xi_r} \quad (23)$$

Integration of the above equation over both sides of the flame results in

$$\left[\left(\frac{d \theta_r}{d \xi_r} \right)^2 \right]_{-\infty}^{0-} = 2 q_{rf} \epsilon_r \exp(\eta_f^2) T_f \quad (24)$$

$$\left[\left(\frac{d \theta_r}{d \xi_r} \right)^2 \right]_{0+}^{\infty} = -2 q_{rf} \epsilon_r \exp(\eta_f^2) T_f \quad (25)$$

where $[\phi]_a^b$ denotes $[\phi]_b - [\phi]_a$ and $[\phi]_a$ stands for the value of ϕ evaluated at a .

Reaction Zone

In the reaction zone, radiation and convection can be neglected and the governing equations are

$$\frac{d^2 T}{d \eta^2} = \omega \quad (26)$$

$$\frac{1}{Le_F} \frac{d^2 Y_F}{d \eta^2} = -\omega \quad (27)$$

$$\frac{1}{Le_O} \frac{d^2 Y_O}{d \eta^2} = -\omega \quad (28)$$

By combining Eqs. 26 and 27 and using the assumption that the Lewis number is only different from unity in $O(\epsilon)$, the following jump condition across the flame can be obtained as

$$\left[\frac{dT}{d\eta} \right]_{\eta_f^-}^{\eta_f^+} + \frac{1}{Le_F} \left[\frac{dY_F}{d\eta} \right]_{\eta_f^-}^{\eta_f^+} = 0 \quad (29)$$

While combination of Eqs. 27 and 28 results in the jump condition of mass fraction gradients across the flame

$$\frac{1}{Le_O} \left[\frac{dY_O}{d\eta} \right]_{\eta_f^-}^{\eta_f^+} = \frac{1}{Le_F} \left[\frac{dY_F}{d\eta} \right]_{\eta_f^-}^{\eta_f^+} \quad (30)$$

Substitution of the outer solutions given in Eqs. 10, 11, 13, and 14 into Eq. 30 yields

$$\begin{aligned} & \frac{Y_{F,-\infty} \exp\left(-Le_F \frac{1}{2} \eta_f^2\right)}{Le_F \int_{-\infty}^{\eta_f} \exp\left(-Le_F \frac{1}{2} t^2\right) dt} \\ &= \frac{Y_{O,\infty} \exp\left(-Le_O \frac{1}{2} \eta_f^2\right)}{Le_O \int_{\eta_f}^{\infty} \exp\left(-Le_O \frac{1}{2} t^2\right) dt} \end{aligned} \quad (31)$$

The above equation determines the flame location η_f , which is the same as that derived by Chung and Law [3] for counterflow diffusion flames without radiation heat loss.

Using the outer solution of Y_F given in Eqs. 10 and 13, the temperature jump across the flame can be found from Eq. 29 to be,

$$\left[\frac{dT}{d\eta} \right]_{\eta_f^-}^{\eta_f^+} = - \frac{Y_{F,-\infty}}{Le_F \int_{-\infty}^{\eta_f} \exp \left(-Le_F \frac{1}{2} t^2 \right) dt} \exp \left(-Le_F \frac{1}{2} \eta_f^2 \right) \quad (32)$$

Note that the outer temperature solutions given in Eqs. 9 and 12 cannot be substituted into the left-hand side of the above equation since these solutions are not valid in the vicinity of the reaction zone due to the effect of radiation heat loss [6]. Insertion of outer temperature solutions to the left-hand side of Eq. 32 leads to the determination of the adiabatic flame temperature.

From Eqs. 19, 20, and 15, one has

$$\frac{d\theta_r}{d\xi_r} = \frac{dT}{dz} = \frac{dT}{d\eta} \frac{d\eta}{dz} = \frac{dT}{d\eta} \exp \left(\frac{1}{2} \eta_f^2 \right) \quad (33)$$

By using the above equation and matching with the outer temperature solution given in Eq. 9, one has

$$\left[\frac{d\theta_r}{d\xi_r} \right]_{-\infty} = \exp \left(\frac{1}{2} \eta_f^2 \right) \left[\frac{dT}{d\eta} \right]_{\eta_f^- - O(\epsilon_r)} = \frac{T_f - T_{-\infty}}{\int_{-\infty}^{\eta_f} \exp \left(-\frac{1}{2} t^2 \right) dt} \quad (34)$$

where $\eta_f^- - O(\epsilon_r)$ denotes the boundary between the outer zone and the radiation zone on the fuel side (Fig. 1). Substitution of Eq. 34 into Eq. 24 leads to

$$\left[\frac{d\theta_r}{d\xi_r} \right]_{0^-} = F_F(\eta_f, T_f, T_{-\infty}) \quad (35)$$

where

$$F_F(\eta_f, T_f, T_{-\infty}) = \sqrt{2q_{rf}\epsilon_r T_f \exp(\eta_f^2) + \left(\frac{T_f - T_{-\infty}}{\int_{-\infty}^{\eta_f} \exp \left(-\frac{1}{2} t^2 \right) dt} \right)^2} \quad (36)$$

Similarly, it can be shown that

$$\left[\frac{d\theta_r}{d\xi_r} \right]_{0^+} = -F_O(\eta_f, T_f, T_{\infty}) \quad (37)$$

where

$$F_O(\eta_f, T_f, T_{\infty}) = \sqrt{2q_{rf}\epsilon_r T_f \exp(\eta_f^2) + \left(\frac{T_f - T_{\infty}}{\int_{\eta_f}^{\infty} \exp \left(-\frac{1}{2} t^2 \right) dt} \right)^2} \quad (38)$$

It can be shown from Eq. 32, using Eqs. 33, 35, and 37, that

$$F_F(\eta_f, T_f, T_{-\infty}) + F_O(\eta_f, T_f, T_{\infty}) = \frac{Y_{F,-\infty} \exp \left(\frac{1}{2} (1 - Le_F) \eta_f^2 \right)}{Le_F \int_{-\infty}^{\eta_f} \exp \left(-Le_F \frac{1}{2} t^2 \right) dt} \quad (39)$$

In the above equation, the left-hand side terms represent heat conduction and radiation heat loss from both sides of the flame. The right-hand side stands for heat release due to chemical reaction.

Analysis of Extinction

In order to perform analysis of extinction, it is necessary to investigate the structure of the reaction zone. It should be emphasized that the following simplified extinction analysis is valid only for an $O(\epsilon)$ deviation of Lewis numbers from unity. Otherwise, the extinction criterion would be dependent on the amount of reactant leakage through the flame. Inside the reaction zone, the flame temperature and mass fractions of fuel and oxidizer can be expanded using the small parameter ϵ as follows

$$T = T_f - \epsilon \theta \quad (40)$$

$$Y_F = \epsilon y_F \quad (41)$$

$$Y_O = \epsilon y_O \quad (42)$$

By introducing an inner stretched coordinate

$$\xi = \frac{\eta - \eta_f}{\epsilon A} \quad (43)$$

where A is a constant to be determined, the reaction zone energy and species equations can be written as

$$\frac{d^2\theta}{d\xi^2} = -\epsilon\omega A^2 = \epsilon D_a Y_O Y_F \exp\left(-\frac{T_a}{T}\right) A^2 \quad (44)$$

$$\frac{1}{Le_F} \frac{d^2 y_F}{d\xi^2} = -\epsilon\omega A^2 \quad (45)$$

$$\frac{1}{Le_O} \frac{d^2 y_O}{d\xi^2} = -\epsilon\omega A^2 \quad (46)$$

Using Eqs. 40 and 43, one has

$$\frac{d\theta}{d\xi} = -A \frac{dT}{d\eta} \quad (47)$$

Thus, boundary condition for Eq. 44 at negative infinity can be obtained by substituting Eqs. 33 and 35 into Eq. 47

$$\left[\frac{d\theta}{d\xi}\right]_{-\infty} = -A \exp\left(-\frac{1}{2} \eta_f^2\right) F_F(\eta_f, T_f, T_{-\infty}) \quad (48)$$

The boundary condition at positive infinity can be similarly obtained

$$\left[\frac{d\theta}{d\xi}\right]_{\infty} = A \exp\left(-\frac{1}{2} \eta_f^2\right) F_O(\eta_f, T_f, T_{\infty}) \quad (49)$$

By selecting A as

$$A = \left[\frac{Y_{F,-\infty} \exp\left(-\frac{1}{2} Le_F \eta_f^2\right)}{Le_F \int_{-\infty}^{\eta_f} \exp\left(-\frac{1}{2} Le_F t^2\right) dt} \right]^{-1} \quad (50)$$

Eq. 48 takes the form

$$\left[\frac{d\theta}{d\xi}\right]_{-\infty} = -m \quad (51)$$

where

$$m = \frac{F_F(\eta_f, T_f, T_{-\infty})}{Y_{F,-\infty} \exp\left[\frac{1}{2} (1 - Le_F) \eta_f^2\right]} \quad (52)$$

$$Le_F \int_{-\infty}^{\eta_f} \exp\left(-\frac{1}{2} Le_F t^2\right) dt$$

is the ratio of heat loss from the flame to the fuel side to the heat release due to chemical reaction. Equation 49 now becomes

$$\left[\frac{d\theta}{d\xi}\right]_{\infty} = -m + 1 \quad (53)$$

Substitution of Eq. 45 into Eq. 44 results in

$$\frac{d^2\theta}{d\xi^2} = \frac{1}{Le_F} \frac{d^2 y_F}{d\xi^2} \quad (54)$$

Integration of Eq. 54 along with the use of boundary condition Eq. 53 yields

$$y_F = Le_F [\theta + (m - 1)\xi] \quad (55)$$

Insertion of Eq. 46 into Eq. 44 leads to

$$\frac{d^2\theta}{d\xi^2} = \frac{1}{Le_O} \frac{d^2 y_O}{d\xi^2} \quad (56)$$

Integration of Eq. 56 using the boundary condition given in Eq. 51 yields

$$y_O = Le_O (\theta + m\xi) \quad (57)$$

Substitution of Eqs. 40, 55, and 57 into Eq. 44 results in

$$\frac{d^2\theta}{d\xi^2} = \Lambda (\theta + m\xi) [\theta + (m - 1)\xi] \exp(-\theta) \quad (58)$$

where

$$\Lambda = \epsilon^3 D_a Le_O Le_F A^2 \exp\left(-\frac{T_a}{T_f}\right) \quad (59)$$

is the reduced Damköhler number. It is worth noting that the reduced Damköhler number has the same form as that given by Chung and Law [3] in the limit of $Le_i = 1 + O(\epsilon)$. By further defining

$$\Psi = (4\Lambda)^{1/3} \left[\theta + (2m - 1) \frac{\xi}{2} \right] \quad (60)$$

$$\psi = (4\Lambda)^{1/3} \frac{1}{2} \xi \quad (61)$$

it can be shown that the energy equation given in Eq. 58 takes the following form

$$\frac{d^2\Psi}{d\psi^2} = (\Psi + \psi)(\Psi - \psi) \exp\{- (4\Lambda)^{-1/3} [\Psi + (2(1 - m) - 1)\psi]\} \quad (62)$$

The corresponding boundary conditions, Eqs. 51 and 53, reduce to

$$\frac{d\Psi}{d\psi} = -1 \quad \text{as } \psi \rightarrow -\infty \quad (63)$$

$$\frac{d\Psi}{d\psi} = 1 \quad \text{as } \psi \rightarrow \infty \quad (64)$$

The boundary value problem defined by the above three equations has been solved by Liñán [1] who provided an excellent approximation for the reduced Damköhler number at extinction [1, 6]

$$\Lambda_e = \frac{ec}{2} (1 - 2c + 1.04c^2 + 0.44c^3) \quad (65)$$

where

$$c = \min(m, 1 - m) \quad (66)$$

Extinction is expected to occur if $\Lambda < \Lambda_e$.

It is interesting to note that the structure equations of the reaction zone, Eqs. 51, 53, and 58, derived under the conditions of the present analysis (with radiation heat loss from the flame and nonunity Lewis numbers) can still be cast into the same form, Eqs. 61–63, as those obtained from all the previous studies of quasi-steady, adiabatic or nonadiabatic, unity Lewis numbers or nonunity Lewis numbers. This observation has been made and discussed extensively by Chao and Law [12].

RESULTS AND DISCUSSION

The starting point of the numerical calculation is to search for the flame location η_f . The flame location is obtained iteratively by solving Eq. 31 using the algorithm described as follows. Using a guessed flame location, η_f^* , the integration $\int_{-\infty}^{\eta_f^*} \exp(-Le_F \frac{1}{2} t^2) dt$ is first calculated. This then allows the integration $\int_{\eta_f^*}^{\infty} \exp(-Le_O \frac{1}{2} t^2) dt$ to be evaluated using Eq. 31. The flame location can therefore be updated based on the value of $\int_{\eta_f^*}^{\infty} \exp(-Le_O \frac{1}{2} t^2) dt$. Iteration continues until the change of the flame location is sufficiently small.

Once the flame location is found, the flame temperature is calculated next. For a given stretch rate, the flame temperature is calculated

iteratively by solving Eq. 39. Various iteration schemes were tested. They encountered difficulties at small stretch rates. The following surprisingly simple scheme offers fast and stable convergence without any difficulties

$$T_f = T_f^* + \frac{Y_{F,-\infty} \exp\left(\frac{1}{2}(1 - Le_F)\eta_f^2\right)}{Le_F \int_{-\infty}^{\eta_f} \exp\left(-Le_F \frac{1}{2} t^2\right) dt} - F_F(\eta_f, T_f^*, T_{-\infty}) - F_O(\eta_f, T_f^*, T_{\infty}) \quad (67)$$

where T_f^* is the guessed flame temperature. To analyze flame extinction, it is easier to find the extinction stretch rates by plotting the reduced Damköhler number, Eq. 59, and the extinction Damköhler number, Eq. 65, as a function of the stretch rate on the same graph. In general, there are three scenarios. First, the two curves have two interception points. The interception point at the higher stretch rate defines the conventional quenching limit due to a too short residence time and the point at the lower stretch rate corresponds to the radiation extinction limit due to excessive radiation heat loss. Secondly, the two curves have one interception point which represents the merger of the quenching and radiation extinction limits. This point also defines the flammability limit and the stretch rate associated with this limit. Thirdly, the two curves have no interception points, which implies that steady-state burning is not possible.

The following parameters are used in all the numerical calculations: $T_a = 0.9$, $\gamma = 4$, $\bar{K}_p = 1 \text{ m}^{-1}$, $k = 2$, $\bar{c}_p = 1400 \text{ J/kg}$, $\bar{T}_{-\infty} = 300 \text{ K}$, $\bar{T}_{\infty} = 300 \text{ K}$, $\bar{\rho} = 0.8 \text{ kg/m}^3$, $\epsilon_r = 0.25$, $\bar{B} = 2.4 \times 10^{10} \text{ m}^3/\text{mol s}$, and $\bar{M}_F = 0.016 \text{ kg/mol}$. These parameters simulate methane–air combustion in a rough sense. Unless otherwise stated, all the results were obtained with radiation heat loss.

To illustrate how the extinction conditions are determined, Fig. 2 shows the reduced Damköhler number and the extinction Damköhler number as a function of the stretch rate for $Le_F = 1$, $Le_O = 1$, $\bar{Y}_F = 1$, and $\bar{Y}_O = 0.192$. It will be seen later that these conditions

Fig. 2. Variation of the reduced and extinction Damköhler numbers with the stretch rate with and without radiation heat loss: $Le_F = 1$, $Le_O = 1$, $\bar{Y}_F = 1$, $\bar{Y}_O = 0.192$. Also shown in this figure are the flame temperatures with radiation (filled triangles) and without radiation (open triangles).

are close to the flammability limit in terms of the oxygen concentration when radiation is considered. When radiation is taken into account, the reduced Damköhler number first increases as the stretch rate decreases then starts to decrease as the stretch rate further decreases, while the extinction Damköhler number monotonically increases with decreasing the stretch rate. Under these conditions, the two curves have two intercept points, corresponding to respectively the radiation extinction at a lower stretch rate, about 2.2 s^{-1} , and the conventional quenching at a higher stretch rate, about 10 s^{-1} . Without radiation heat loss, however, the picture is quite different. The reduced Damköhler number increases sharply as the stretch rate decreases. The extinction Damköhler number remains constant due to constant heat loss to the fuel side through heat conduction. The two curves have only one intercept point at about 31 s^{-1} , defining the quenching condition. When radiation is considered and the oxygen mass fraction is reduced to 0.191, the two curves have only one intercept point. This situation defines two critical values: the critical oxygen concentration (0.191) below which steady-state combustion cannot be sustained, and the critical stretch rate above or below which steady-state combustion is again not sustainable.

To assist the discussions of the effects of Lewis numbers on flame location and flame temperature, variations of $H_F(Y_{F,-\infty}, Le_F,$

Fig. 3. Variation of $H_F(Y_{F,-\infty}, Le_F, \eta) = Y_{F,-\infty} \exp(\frac{1}{2}(1 - Le_F)\eta^2)/Le_F \int_{-\infty}^{\eta} \exp(-Le_F \frac{1}{2}t^2) dt$ and $H_O(Y_{O,\infty}, Le_O, \eta) = Y_{O,\infty} \exp(\frac{1}{2}(1 - Le_O)\eta^2)/Le_O \int_{-\infty}^{\eta} \exp(-Le_O \frac{1}{2}t^2) dt$ with η for different Lewis numbers: $\bar{Y}_F = 1$, $\bar{Y}_O = 0.23$.

$\eta) = Y_{F,-\infty} \exp(\frac{1}{2}(1 - Le_F)\eta^2)/Le_F \int_{-\infty}^{\eta} \exp(-Le_F \frac{1}{2}t^2) dt$ and $H_O(Y_{O,\infty}, Le_O, \eta) = Y_{O,\infty} \exp(\frac{1}{2}(1 - Le_O)\eta^2)/Le_O \int_{-\infty}^{\eta} \exp(-Le_O \frac{1}{2}t^2) dt$ with η are shown in Fig. 3 for $\bar{Y}_{F,-\infty} = 1.0$, $\bar{Y}_{O,\infty} = 0.23$, and different Lewis numbers. Based on Eq. 31, the intercept point of $H_F(Y_{F,-\infty}, Le_F, \eta)$ and $H_O(Y_{O,\infty}, Le_O, \eta)$ curves defines the flame location η_f . In addition, $H_F(Y_{F,-\infty}, Le_F, \eta)$ or $H_O(Y_{O,\infty}, Le_O, \eta)$ represents combustion heat release, Eqs. 31 and 39. Under the conditions of $\bar{Y}_{F,-\infty} = 1.0$ and $\bar{Y}_{O,\infty} = 0.23$, variation of the fuel Lewis number has a much greater effect on $H_F(Y_{F,-\infty}, Le_F, \eta)$ than that of Le_O on $H_O(Y_{O,\infty}, Le_O, \eta)$. This is simply because the constant factor in $H_O(Y_{O,\infty}, Le_O, \eta)$, $Y_{O,\infty}$, is much smaller than that in $H_F(Y_{F,-\infty}, Le_F, \eta)$, $Y_{F,-\infty}$. Physically, it corresponds to the fact that per unit mass of fuel requires a much larger amount of oxidizer to react completely. It is clear from the results shown in Fig. 3 that the fuel stream Lewis number has a much stronger impact on the flame location and heat release than the oxidizer Lewis number.

Figure 4 displays the flame location as a function of the oxygen mass fraction for $\bar{Y}_{F,-\infty} = 1.0$ and different oxidizer and fuel Lewis numbers. Departure of the fuel Lewis numbers from unity has a much stronger effect on the flame location than the oxidizer Lewis numbers, as has been anticipated from the results shown in Fig. 3. Flame moves closer to

Fig. 4. Effects of the oxygen concentration and the fuel and oxidizer Lewis numbers on the flame location: $\bar{Y}_F = 1$.

the stagnation point as the oxygen concentration increases, a consequence of the stoichiometric condition. Figure 5 shows the variation of the nondimensional adiabatic flame temperature with oxygen mass fraction for different fuel and oxidizer Lewis numbers. The adiabatic flame temperature increases with increasing the oxygen mass fraction due to the following two reasons. First, increasing the oxygen mass fraction results in higher combustion heat release, which can be realized based on the results shown in Fig. 3, since the $H_O(Y_{O,\infty}, Le_O, \eta)$ curves move toward the left. Second, the heat conduction loss from the flame to the oxidizer side, which is dominant to the heat conduction loss to the fuel side, decreases as the flame moves toward the stagnation plane with increasing the oxygen mass fraction. Although lowering

Fig. 5. Effects of the oxygen concentration and the fuel and oxidizer Lewis numbers on the nondimensional adiabatic flame temperature: $\bar{Y}_F = 1$.

Fig. 6. Variation of the nondimensional flame temperature with the stretch rate for different Lewis numbers of the fuel and oxidizer streams: $\bar{Y}_F = 1$, $\bar{Y}_O = 0.23$.

both the fuel Lewis number and the oxidizer Lewis number results in higher adiabatic flame temperature, the mechanisms are quite different. Decreasing the oxidizer Lewis number in general leads to a slightly higher heat release and reduced heat conduction loss to the oxidizer side as the flame moves closer to the stagnation plane (Fig. 3). As a result, the adiabatic flame temperature increases. In contrast, reduction of the fuel Lewis number has two opposite effects on the flame temperature. On the one hand the results shown in Fig. 3 suggest that the heat release increases with decreasing the fuel Lewis number. On the other hand, as the fuel Lewis number decreases the flame moves further away from the stagnation plane toward the oxidizer stream which increases the conduction heat loss from the flame to the oxidizer side. The increased flame temperature with decreasing the fuel Lewis number is therefore due to a stronger increase of the heat release than that of the conduction heat loss. Results shown in Fig. 5 indicate that for the same derivation from unity the oxidizer Lewis number has a slightly stronger effect on the flame temperature than the fuel Lewis number. The adiabatic flame temperature increases almost linearly with the oxygen concentration.

Figure 6 shows the nondimensional flame temperature as a function of the stretch rate for different Lewis numbers of the oxidizer and the fuel streams. Note that the ending points of each curve on both sides represent the corresponding extinction conditions. Deviation of the

Fig. 7. Variation of the stretch rate at extinction with the oxygen concentration for three different oxidizer Lewis numbers: $Le_F = 1$, $\bar{Y}_F = 1$.

oxidizer Lewis number from unity has a stronger effect on the flame temperature than that of the fuel Lewis number, especially at high stretch rates. It is interesting to see that this difference vanishes near the radiation extinction limits. The greater effects of Lewis numbers on the flame temperature at high stretch rates reflect the more dominant role of conduction heat loss. On the other hand, Lewis numbers have a smaller effect on the flame temperature at small stretch rates, since in this limit radiation heat loss dominates heat conduction. Smaller Lewis numbers of the fuel or the oxidizer lead to higher flame temperature, similar to the results given in Fig. 5.

Variations of the extinction stretch rate as a function of the oxygen mass fraction for different Lewis numbers of the oxidizer are shown in Fig. 7. The upper branch of the C-shaped curve corresponds to the quenching limit and the lower branch stands for the radiation extinction limit. The merging point of the two branches defines the flammability limit in terms of the oxygen concentration for the given fuel concentration. Lower oxidizer Lewis numbers result in lower flammability limit of oxygen concentration. This may be attributed to the higher flame temperature which has a strong impact on the flame structure and extinction through the exponential reaction term. A similar C-shaped extinction curve to that shown in Fig. 7 has been previously obtained by T'ien [7] in a study of the effects of surface radiation on diffusion flame in the stagnation point region of a condensed fuel.

Fig. 8. Variation of the stretch rate at extinction with the fuel concentration for different fuel Lewis numbers: $\bar{Y}_O = 0.23$.

Figure 8 shows the variation of the extinction stretch rate as a function of the fuel concentration for different fuel and oxidizer Lewis numbers. Once again, this is a C-shaped curve with the upper branch defining the quenching limit and the lower branch identifying the radiation extinction limit. The merging point of the two branches defines the flammability limit in terms of the fuel concentration. A similar C-shaped extinction curve for counterflow diffusion methane flame has been obtained both experimentally and numerically by Maruta et al. [11]. Similar to the results shown in Fig. 7, a smaller fuel Lewis number leads to a lower flammability limit (lower fuel concentration at the merging point). This is again due to the higher flame temperature at lower Lewis numbers (Fig. 6). The extinction curve for $Le_O = 0.9$ and $Le_F = 1.1$ is almost identical with that for $Le_O = 1.0$ and $Le_F = 1.0$.

Variations of the flame location with the fuel concentration for different fuel and oxidizer Lewis numbers are shown in Fig. 9. Fuel Lewis number has a stronger effect on the flame location, as has already been observed in Fig. 4. This effect becomes less significant as the fuel concentration decreases. This is because as the fuel mass fraction decreases, the flame moves closer to the stagnation plane. Figure 10 shows the variation of the nondimensional adiabatic flame temperature with the fuel mass fraction for different fuel and oxidizer Lewis numbers. Departure of the oxidizer Lewis number from unity is more effective than the fuel Lewis

Fig. 9. Effects of the fuel concentration and fuel and oxidizer Lewis numbers on the flame location: $\bar{Y}_O = 0.23$.

number in affecting the flame temperature at high fuel concentration. At low fuel concentrations, the same deviations of the fuel and oxidizer Lewis numbers from unity yield almost the same adiabatic flame temperature.

Figure 11 shows the flammable boundary for the counterflow diffusion flame. It should be pointed out that these results can only be treated as qualitative but not quantitative primarily due to the constant density assumption made in the present analysis. Larger Lewis numbers (either oxidizer or fuel streams) lead to smaller flammable region and smaller Lewis numbers increase the flammable region. This is the expected effect of Lewis number based on its effect on flame temperature. Although the present analysis is limited to small deviation of Lewis numbers from unity, it may be anticipated

Fig. 10. Effects of the fuel concentration and the fuel and oxidizer Lewis numbers on the nondimensional adiabatic flame temperature: $\bar{Y}_O = 0.23$.

Fig. 11. Boundary of the flammable and nonflammable region in the fuel and oxygen space for three oxidizer Lewis numbers: $Le_F = 1$.

from the trend of the results shown in Fig. 11 that the point ($\bar{Y}_F = 1, \bar{Y}_O = 0.23$), which corresponds to counterflow of pure fuel (methane in this case) and air, may fall in the non-flammable region, i.e., steady-state burning is not possible, if the Lewis numbers of the oxidizer and fuel are sufficiently large.

CONCLUSIONS

Effects of radiation heat loss and minor perturbations in the Lewis number on the structure and extinction of diffusion flame established near the stagnation point of two opposed streams of fuel and oxidizer have been analyzed using the asymptotic method of large activation energy for small deviation of the fuel and oxidizer Lewis numbers from unity. The analysis successfully predicts the existence of two extinction limits when radiation heat loss from the flame is considered. The C-shaped extinction curves in both the oxygen and fuel concentration space revealed in previous studies have also been reproduced. Lewis numbers of fuel and oxidizer affect both the flame location and the flame temperature. Consequently, they affect the extinction limits and flammability limits of counterflow diffusion flames.

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