Preferential diffusion effects for laminar flame in a co-flow mixing layer with widely varying Lewis number and Lewis numbers greater than unity.

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Abstract
Here, the previous work on oscillatory behavior of laminar flames with varying premixedness is expanded by relaxing the equal Lewis number assumption. The Lewis number of fuel and oxidizer is varied separately. And the simulation are run for co-flow mixing layer, where fuel rich stream and oxidizer rich stream with a given premixedness is allowed to mix and burn, thus giving rise to a flame. This flame shape varies from pure diffusion (trailing edge flame for premixedness of zero to plane premixed flame for premixedness of unity (fully premixed mixture). Initially the Lewis number of fuel and oxidizer were kept constant. When the Lewis number of fuel and oxidizer is varied individually, various long term behaviors like steady state or limit cycle oscillations was observed. These are presented as contour plots of amplitude of heat release reaction rate oscillations in Lewis number of fuel-Lewis number of oxidizer plane, for different premixedness. It is found that the constant amplitude lines are almost linear for diffusion flame and partially premixed flames validating the effective Lewis number definition hitherto defined for diffusion flames. But for near premixed flames there is significant variation, where the constant amplitude lines are curved. Also the amplitude of oscillations are much higher for near premixed flames than for other flames. The change in structure of the flame from symmetric triple flame to asymmetric triple flame and change in triple point is also observed. Change of this asymmetricity for different premixedness is also presented.

Introduction

In many practical combustion applications, unstable behavior in the combustion chamber may lead some systems to fail, leading to disaster. This unstable behavior in the combustion chamber can be characterized by unstable flame behaviors. This may be due to many physical causes viz., flow instabilities, Hydrodynamic instability, Thermo-diffusive instability, Kelvin Helmholtz instability, buoyancy effects etc. Now at some particular unstable behavior may be caused due to one or more effects dominating the others. Thus, in order to know the actual mechanism behind a behavior, one need to study the characteristics of these physical mechanisms separately and their interactions with each other. Since thermo-diffusive mechanism is basic to many combustion systems, it is of more importance and is considered here. It is believed that that cellular instability occurs for both premixed and non-premixed flames for Lewis numbers less than unity and pulsating instabilities occur for Lewis number greater than unity. The critical Lewis number is found to be in the range (1.5 to 2.2) which varies with equivalence ratio, heat loss, premixedness etc [1].

Many theoretical studies have been carried out for equal Lewis number for both premixed flames and diffusion flames. In most of the recent combustion systems, Lewis number of fuel significantly differs from oxidizer. This is also critical to stability of a flame. Since, we have observed a stability map from the flame with equal Lewis number. Now in case of unequal Lewis number the criteria for stability is in question, whether to take into account Lewis number of fuel or oxidizer. Generally in case of off-stoichiometric reactants compositions, (rich or lean), the Lewis number of one of the reactants plays a dominant role. But in this case of ϕ = 1, both the Lewis number may play a role.Very few studies have been carried out for laminar flames with these preferential diffusion effects.

It is reported that preferential diffusion effects significantly increase the propensity for instability in premixed flames with increase in the Markstein length [2]. In a diffusion flame formed by co-flow burner experiments [3], it is shown that the onset of oscillations can be characterized by an effective Lewis number which is defined as the weighted combination of Lewis numbers of both reactants. Further pulsating oscillations have been proven to occur if this effective Lewis number is greater than or equal to 2.6

A Theoritical study for this type of configuration is not reported to our knowledge. However for a strained-diffusion flame in a counter-flow configuration theoretical studies under the framework of Thermo-diffusive model have indicated that for effective Lewis number greater than 2.2, pulsating oscillations are likely to occur [4]. Nevertheless for partially premixed flames, effects of preferential diffusion on pulsating behavior have not yet reported.

Previous study [5] on laminar flames in a co-flow with equal Lewis number of reactants have shown that there is stability regime for low Damköhler numbers and mid range of premixedness, that show onset of pulsating instability at Le=1.5. Also premixed flames show pulsating behavior for Lewis numbers greater than 1.6. This work is extended to understand the stability behavior for unequal Lewis number in the full range of premixedness.

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Theoretical Formulation

To simulate actual conditions in the practical situations, configuration wherein a semi-infinite plate of infinitesimal thickness, as shown in Fig. 1, separates two parallel streams of equal velocity u, one of fuel rich mixture with mass fraction profile $Y_{F0}(y)$, and the other of fuel lean mixture with mass fraction profile $Y_{X0}(y)$. It is assumed that thermal conductivity of the plate is sufficiently high so as to maintain its temperature constant and equal to the upstream temperature T_0 of the two streams. Beyond the tip of the plate, fuel and oxidizer inter-diffuse thereby generating a mixing layer. This mixing layer grows downstream and if allowed will be fully mixed at far downstream. When the mixture is ignited successfully, a gas-phase oxidation chemical reaction takes place in the mixing layer. At some distance from the tip of the splitter plate, a flame stands. This flame of an edge from which two segments are attached: a fuel-rich branch extending toward the fuel side and a fuel-lean branch extending toward the oxidizer side. Behind the curved premixed flame front, the unconsumed reactants, which are again of separate origins, are depleted at a diffusion flame that trails behind. The heat conduction back to the relatively cold plate helps to prevent a flashback into the burner. The chemical reaction within the mixture layer is modelled by an overall irreversible one step of the form

$$\nu_F \text{ Fuel} + \nu_X \text{ Oxidizer} \rightarrow (\nu_F + \nu_X) \text{ Product} \qquad (1)$$

where, ν is the number of moles of the species. The fuel consumption rate per unit volume

$$\Omega_F = B\,\rho^2\, Y_F\, Y_X \exp(-E/RT) \qquad (2)$$

is assumed to be of first order with respect to each of the two reactants and obeys the Arrhenius law with a pre-exponential factor B and an overall activation energy E. Here Y_F and Y_X are the mass fractions of fuel and oxidizer, respectively, T and ρ are the temperature and density of the mixture, and R is the gas constant.

We consider a diffusive-thermal model, according to which the density of the mixture ρ, the thermal diffusivity k, the heat capacity Cp, and the individual molecular diffusivities D_F and D_X are all assumed constant. It thus suffices to write down balance equations for the mass fraction of each of the two species and an energy equation for the whole mixture. The mass fractions are normalized with respect to their values in the supply streams, Y_{F0} and Y_{X0}, respectively, and a non-dimensional temperature is introduced, where

$$T = (\tilde{T} - \tilde{T}_0)/\tilde{T}_a - T_0$$

$$\tilde{T}a = \tilde{T}_0 + Q\,(1 + f)\,(\tilde{Y}_{F0} / W_F \nu_F)/Cp \qquad (3)$$

is the adiabatic flame temperature (of the corresponding stoichiometric fuel-air mixture). Here Q is the total heat release and $\phi = (Y_{F0} / W_F\, \nu_F)/(Y_{X0}/ W_X\, \nu_X)$ the overall mixture equivalence ratio.

The equations are non-dimensionalised using a thermal diffusive convective length scale ($l_T = \alpha / u$) and associated time scale (l_T / u) with the uniform inlet velocity u.

$$\left.\begin{aligned}
&\frac{\partial T}{\partial t} + \frac{\partial T}{\partial x} - \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = \omega(1+\phi)\\
&\frac{\partial Y_F}{\partial t} + \frac{\partial Y_F}{\partial x} - \frac{1}{Le}\left(\frac{\partial^2 Y_F}{\partial x^2} + \frac{\partial^2 Y_F}{\partial y^2}\right) = -\omega\\
&\frac{\partial Y_X}{\partial t} + \frac{\partial Y_X}{\partial x} - \frac{1}{Le}\left(\frac{\partial^2 Y_X}{\partial x^2} + \frac{\partial^2 Y_X}{\partial y^2}\right) = -\phi\,\omega
\end{aligned}\right| \qquad (4)$$

$$\omega = Da\,\beta^3 Y_F Y_X \exp\left(\frac{\beta(T-1)(1+\gamma)}{(1+\gamma T)}\right) \qquad (5)$$

$$Da = B\,\rho\, Y_{X0} \exp(-E_A / RT_a) / \beta^3 \qquad (6)$$

where, $\phi = \frac{Wx\,\nu_x}{Yx0} / \frac{W_f\,\nu_f}{Yf0}$ is the far field inlet equivalence ratio.

With following boundary conditions

$$T\big|_{x=0} = 0 \qquad Y_F\big|_{x=0} = Y_{F0}(y,\zeta)$$

$$Y_X\big|_{x=0} = Y_{X0}(y,\zeta) \qquad \left.\frac{\partial Y_F}{\partial y} = \frac{\partial Y_X}{\partial y} = \frac{\partial \theta}{\partial y}\right|_{y=\pm L} = 0 \qquad (7)$$

Where, Y_{F0} and Y_{X0} assume the typical profile based on the value of premixedness parameter ζ.

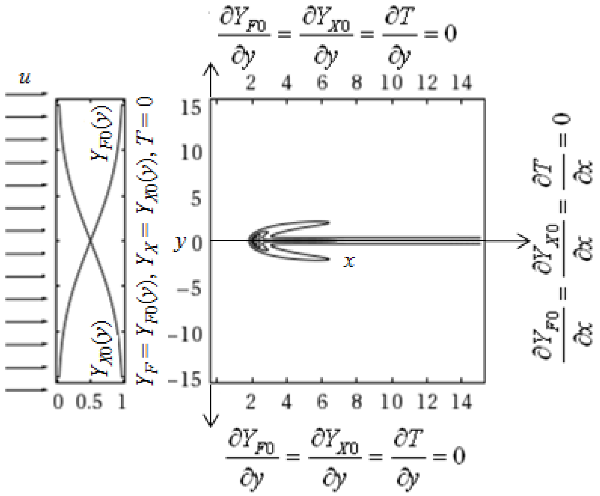

Figure 1: Schematic of the non-dimensional physical and computational domains, inlet flow, and boundary conditions.

Premixedness parameter

The structure of the flame and its stability depends on the inlet reactants concentration profile. The inlet profiles of the fuel and oxidizer mass fractions decide the mixedness of the inlet fuel-oxidizer mixture. Spatially uniform mass fractions of both the reactants imply a fully premixed mixture. This would yield a pure premixed flame. The inlet profile corresponding to completely unmixed reactants would be a step function for both reactants, which would give a pure diffusion flame.

However, the inlet profiles for partially premixed flames lie in between these two extremes. It is necessary to find a parameter, which when varied, would take the inlet profile between these two extremes.

Here concentration profile at the inlet is chosen from the cold mixing field at certain x-location determined by the premixedness parameter defined as

$$\zeta = \frac{2}{\pi}\cot^{-1}\left(\frac{1}{L}\left\|\nabla Y_{iu}\right\|_{y=0}\right) \quad (8)$$

Here L is characteristic length (here L=15) and Y_{iu} is mass fraction of ith species for the cold mixing field determined by

$$Y_{Fu}(x,y) = Z(x,y,Le_F) \;\; \& \;\; Y_{Xu}(x,y) = 1 - Z(x,y,Le_X)$$

$$Z(\xi,y,Le) = \frac{1}{2} + \frac{Le\,x}{2\pi}\exp\left(Le\xi/2\right)\int_0^y \frac{K_1\left(\frac{Le}{2}\sqrt{\xi^2+\tau^2}\right)}{\sqrt{\xi^2+\tau^2}}\,d\tau \quad (9)$$

Where, K_1 is the modified Bessel Function of first kind.

Using these values a sample profiles are plotted in Figure2

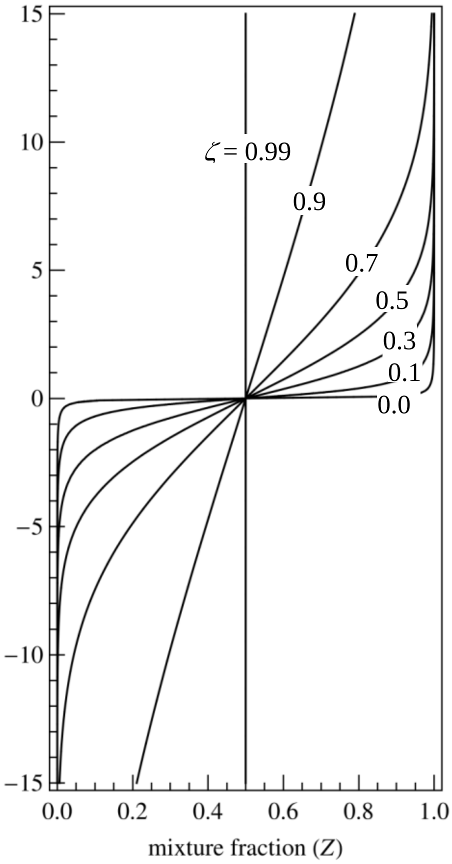

Figure 2: Inlet mixture fraction profiles for various values of premixedness parameter ζ for Le = 1.6.

Numerical Scheme

Numerical scheme closely follows to that of [5]. Equations (4) are solved numerically over a finite domain, 15 x 30 in non-dimensional units. The spatial derivatives are discretized using the 6^{th} order compact scheme at the interior nodes but 4^{th} order at the boundaries of the domain [6].

For temporal integration, 4^{th} order Runge-Kutta time marching is used. This type of numerical scheme is expected to provide spectral-like resolution, which minimizes numerical dissipation effects. The grid is rectangular and uniform, typically with 241 × 481 nodes.

Results and Discussion

Parametric study was carried out to understand the dynamic behavior of flame with varying Lewis number of fuel and oxidizer independently for various values of premixedness. The various parameters and their range considered are as follows:

- Lewis Number of Fuel (Le_F) : (1.0 -1.8)
- Lewis Number of Oxidizer (Le_X) : (1.0 -1.8)
- Premixedness parameter (ζ) : full range (0-1)

Equivalence ratio is assumed to be unity for all cases and Damköhler number is held constant at 100, a mid value where significant amount of oscillations are expected to occur as seen from equal Lewis number simulations reported earlier[5].

For every case the simulation was run using an in-house code. To study the stability, total heat release is considered. Total heat release is calculated by integrating the reaction rate ω over the entire domain. The simulation was run with sufficient low time-step for long time and behavior of heat release was observed. Also field data (T, Y_F, Y_X and ω)are recorded at end of the simulation.

Flame Structure

When Lewis number of Fuel is different from that of the Oxidizer, the flame structure also changes. Fig 3 shows the typical flame structure for the preferential diffusion case where $Le_F < Le_X$.

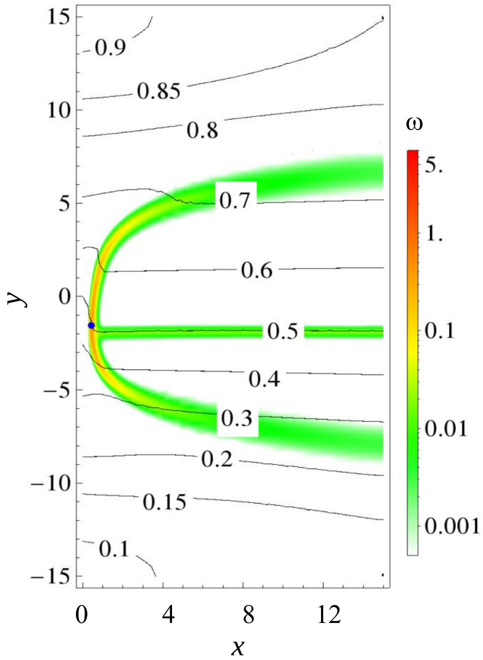

Figure 3: Figure showing density plot of reaction rate field with iso-contours of mixture fraction for premixedness ζ= 0.7 and Le_F = 1.3, Le_X = 1.7.

Here we use iso- contours of mixture fraction (Z) to point the actual stoichiometry line in the reaction rate field.

$$Z = \frac{\phi Y_F - Y_X + 1}{1+\phi}$$

Thus mixture fraction Z = 0.5 corresponds to the stoichiometry. Here we see that unlike in equal Lewis number case, the mixture fraction iso-lines are changed due to presence of flame. Notice at the stoichiometric line shifted from the center line (x = 0) towards the oxidizer side. And the triple point (marked in blue) also gets shifted but lies on the stoichiometric line. Since $Le_F < Le_X$, the fuel diffuses faster into the mixture than oxidizer. Thus the fuel rich area expands into the other side, resulting in the triple point and the diffusion trailing edge shifting to the oxidizer side (y < 0). This results in asymmetric shape of the triple flame. Also the rich premixed branch is larger than lean premixed branch.

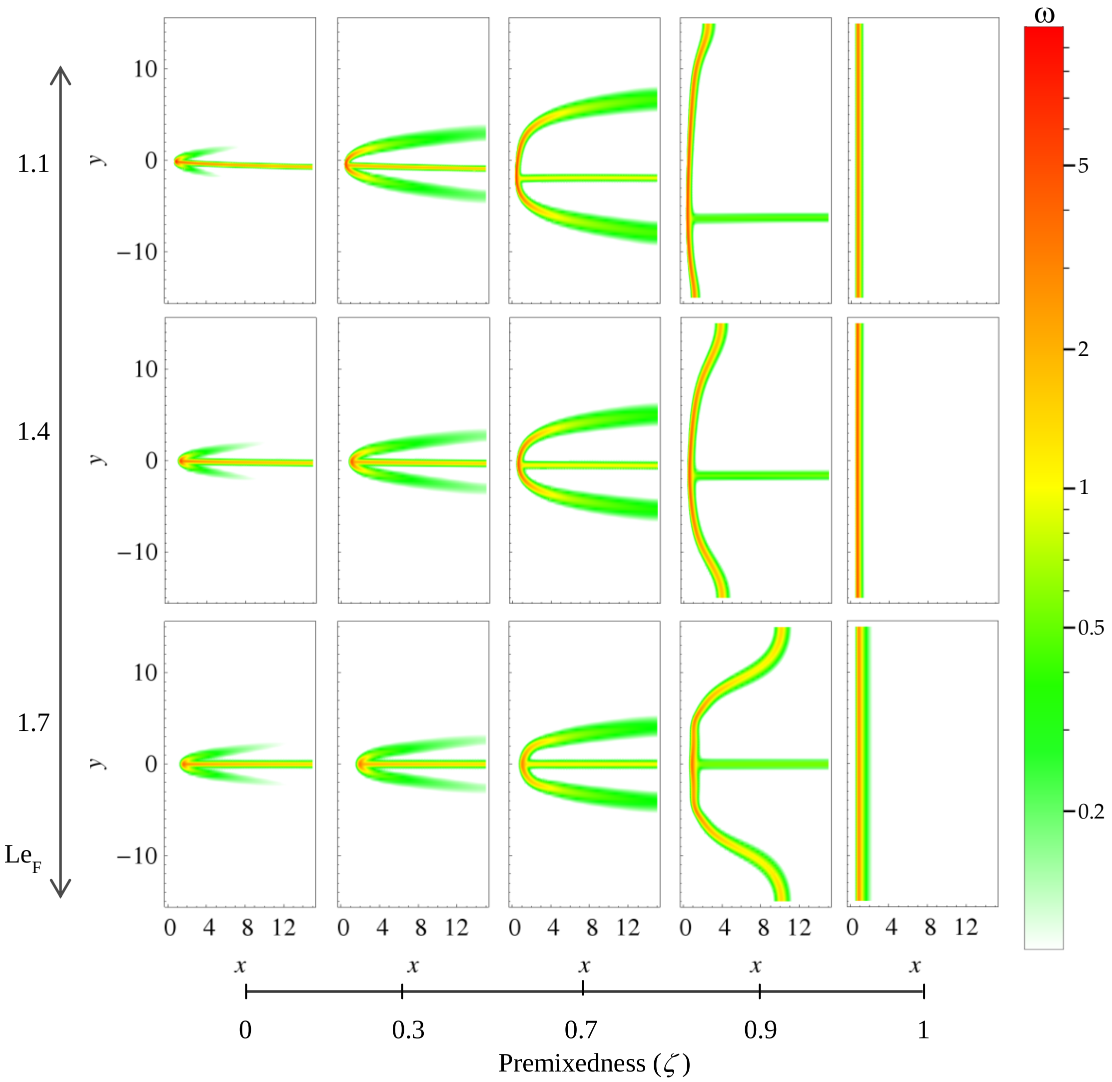

Figure 4 Density plots of reaction rate showing flame structure for different values of premixedness and Fuel Lewis number (with oxidizer Lewis number Le_X = 1.7)

Fig. 4 shows this instantaneous flame structure variation along premixedness and two different Lewis numbers of Fuel with Le_X kept constant along with comparison of equal Lewis number case. As the Lewis number of fuel is decreased from 1.7 implies that the diffusivity of fuel is increased, hence the fuel diffusers faster than oxidizer hence we see a larger premixed branch at the fuel side than at the oxidizer side. This results in asymmetric shape of the triple flame. These effects are milder at Le_F =1.4 and gets significant at Le_F = 1.1, where the disparity between the Lewis number is larger. The flame shifting (or the y-standoff) is mild for low values of premixedness and increases significantly at ζ = 0.9. Even so the asymmetricity and expansion of fuel area also increases with premixedness.

Hence the preferential diffusion affects the premixed flame front with concentration gradient significantly. Larger the front area and larger the disparity between the Lewis number, larger is the effect. As expected preferential diffusion has no asymmetric effect on pure premixed flame nevertheless flame thickness is observed to decrease more apparently in case of premixed flame front.

Flame Stability

Amplitude of heat release is considered as the measure of stability, if the amplitude of heat release is very low or zero, the flame is said to be steady or stable in long-time behavior. Fig 5 shows a iso-contours of amplitude of heat release oscillations plotted in the Lewis number plan i.e. Fuel Lewis Number (Le_F) vs. Oxidizer Lewis Number (Le_X) for Damköhler number (Da) =100.

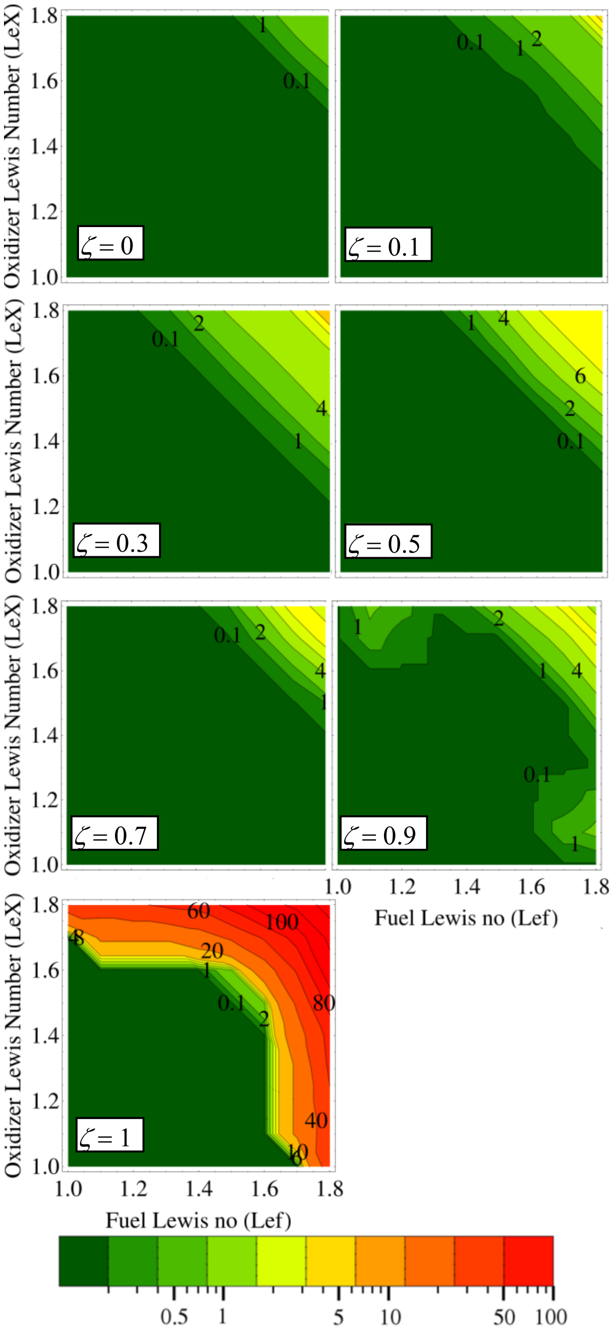

Figure 5 Iso-contours of amplitude of heat release oscillations in Lewis number plane (*LeF-LeX*) for various vales of premixedness (Da = 100)

Here, some interesting results are observed, the flame stability boundary for partially premixed flames is a straight line. Now calculating the equation of straight line it is found that the line satisfies $const = Le_F + Le_X$. Hence from the above results it is inferred that There is some critical value of indicate that there is an effective Lewis number $Le_{eff} = Le_F + Le_X$, such that for Le_{eff} greater dome critical value, the partially premixed flames shows pulsating oscillations. Further it can be conjectured that for off-stoichiometric flames this can be extended as

$$Le_{eff} = \frac{Le_F + \phi Le_X}{1+\phi}.$$

This coincides with previous results [3-4] for diffusion edge flames. Although their work was limited for diffusion flames, from this it can be seen that this is true even for partially premixed flames up to a premixedness of 0.7. Thus the stability boundaries for partially premixed flames can be determined using map as that of equal Lewis nos. using effective Lewis number.

Now this critical Lewis number at which the partially premixed flames show onset of pulsating behavior is high for pure diffusion flame, it decreases and is minimum for around 0.3 and then again increases. Thus partially premixed flames at mid range are susceptible to oscillations at even low effective Lewis number.

Large area of unstable region showing oscillatory behavior is seen for premixedness from 0.9 to unity. Thus Near premixed flames are more prone to instability. Iso-contours of amplitude differ very much from straight line in Lewis number plane. Thus it shows that weighted average value of effective Lewis number does not hold true for premixed flames. Also premixed flames with one of Lewis number as low as 1.1 can show oscillations if the other Lewis number is greater than 1.8. In this respect the partially premixed flames is stable than the premixed flames for the same value of Lewis numbers.

Amplitude of Oscillations

From Fig. 4, one can see that the amplitude of oscillations for partially premixed flames follows the same trend as that of stability map. Thus the lines of constant amplitude matches with that of effective Lewis number for premixedness less than 0.7. Thus for these cases, the amplitude of oscillations also can be determined with use of effective Lewis number. The amplitude of oscillations for partially premixed flame flames (ζ<0.7) peaks at mid value of premixedness (ζ = 0.5) indicating these flames are more propensity of instability.

For premixed flames and near premixed flames the behaviour appears to be non-linear, so no direct relationship for effective Lewis number is proved for now. Nevertheless, equal Lewis number appears to be a representative case. Since premixed flames have more surface are and high heat release, the amplitude of oscillations are one order larger than partially premixed flames.

Conclusions

Thus from the study it can be seen that Preferential diffusion of Fuel and oxidizer in the flame makes the triple flame an asymmetric in shape. Also the triple point along with trailing edge diffusion flame shifts towards reactant side rich in low diffusivity reactant. Premixed flame structure is unaffected by Lewis number disparity except for the thickness.

The stability of the partially premixed and diffusion flames can be determined by use of Effective Lewis number. Thus there is a critical Effective Lewis number for every premixedness at which the onset of pulsating behavior occurs. This critical Lewis number is found to be maximum at premixedness value of 0.3. Thus partially premixed flames at mid range of premixedness have higher propensity for oscillatory behavior.

Premixed flames show oscillatory behavior even if one of the Lewis number is very low at unity and other at 1.8.

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