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Scaling Analysis on Dynamic Flammability Limits of Unsteady Premixed Methane/Air Flames

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A computational study is performed to investigate the effects of mixture composition oscillations on a strained premixed methane/air flame. The problem is of practical relevance in direct-injection spark-ignition (DISI) engines and gas-turbines, in which premixed flames propagate through temporally and spatially stratified mixture field. The primary focus of the study is to identify the dynamic flammability limit, defined as the minimum instantaneous mixture equivalence ratio that can sustain flame propagation. It is shown that the difference between the dynamic and steady flammability limits, $\phi_t - \phi_s$, represents the extension of the flammability limit under unsteady condition, and is a function of the mean strain rate, frequency of oscillation, and mean equivalence ratio. A proper normalization is proposed in order to scale the dynamic flammability limit extension as a function of a nondimensional frequency. As an improvement from previous studies, the use of time scale based on the actual flame thickness and speed represents the correct physical time and length scales involved in the process, thereby yielding a good collapse of the data. As a related subject, a universal extinction criterion for unsteady flames is proposed based on the local Karlovitz number defined as the ratio of the local reaction time to the characteristic flow time. The results show that the maximum local Karlovitz number at the dynamic flammability limit is approximately constant, irrespective of strain rate, mean equivalence ratio, and frequency of oscillation. The results thus extends earlier studies on the local Karlovitz number in steady flame extinction.

Nomenclature

ϕ_s	Steady flammability limit
ϕ_t	Dynamic flammability limit
$\overline{\phi}$	Mean equivalence ratio of oscillation
ϕ_0	Initial equivalence ratio
κ	Imposed flow strain rate
f	Frequency of equivalence ratio oscillation
δ	Thermal flame thickness
τ	Diffusion time based on phase lag
S_L	Laminar flame speed
Ka	Karlovitz number

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I. Introduction

There has been considerable research interest in premixed combustion in a stratified mixture field for its relevance in many practical turbulent combustion systems. For example, in direct-injection spark ignition (DISI) engines, since the fuel is injected directly into the cylinder prior to combustion, there is insufficient time for mixing to homogenize the mixture field prior to the flame propagation. Another application is in gas-turbines where the presence of secondary air and turbulent transport creates an unsteady and nonuniform composition field. Since these spatial and temporal fluctuations involve a wide range of length and time scales, the flame characteristics in such conditions cannot be simply described as a collection of quasi-steady flames. This problem becomes more critical in determining criticality limits. For example, the lean flammability limit for an inhomogeneous mixture depends not only on the amplitude of composition fluctuations, but also on the wave number (or frequency) of the specific modes of fluctuations.

To investigate this isssue, Sankaran and Im[1] studied a one dimensional strained premixed flame subjected to temporal oscillations in the mixture composition. The time-varying response can be readily translated to a spatially non-uniform situation by Eulerian-Lagrangian conversion. The concept of dynamic flammability limit (ϕ_t) was defined as the minimum instantaneous equivalence ratio at which a sustained flame exists. It was observed that, while the steady flammability limit (ϕ_s) is a function of strain rate (κ) alone, the dynamic flammability limit depends also on the mean ($\overline{\phi}$) and frequency (f) of the equivalence ratio oscillation. Moreover, a cut-off frequency beyond which the flame becomes no longer affected by the composition oscillation was identified. Subsequently, a normalized cut-off frequency was proposed by using the steady strain rate as the representative flow time scale. The proposed scaling, however, did not lead to a satisfactory collapse of data for a wide range of parametric conditions, suggesting that an additional time scale may play an important role in characterizing the flame behavior. In an earlier study, Lauvergne and Egolfopoulos[2] alternatively scaled the cut-off frequency with the local flame time ($D/{S_L}^2$) with partial success. Therefore, further consideration is needed in order to explain these observed discrepancies.

The present work thus attempts to revisit this problem more thoroughly. It is conjectured that the main reasons for the data scatters in the dynamic flammability versus frequency curve is the lack of incorporating all relevant physical parameters. In the above two examples, for instance, the steady strain rate does not account for the variations in the mean equivalence ratio. On the other hand, the local flame time is almost independent of strain rate[3] and is mainly a function of mean equivalence ratio only. Therefore, it is clear that neither scaling could simultaneously capture both the characteristic flow and chemical time scales. In this paper, new scaling parameters are introduced based on this consideration, as an anticipation to yield a better collapse of the data and thus a more unified description of the unsteady flame extinction phenomena.

As a related study, Cho *et al*[15] recently demonstrated that a universal extinction criterion can be identified for steady flames in terms of the Karlovitz number based on the local flame quantities. They found that extinction condition for steady premixed flames under various conditions, such as fuel type, equivalence ratio, pressure, and initial temperature, can be determined by the local Karlovitz number. In the present study, it will be shown that the proposed scaling parameter is essentially an extension of this universal steady extinction criterion to unsteady flames. Consequently, the new scaling successfully unifies the lean extinction characteristics of premixed flames, irrespective of strain rate, and mean and frequency of equivalence ratio oscillation.

II. Formulation and Numerical Method

The computational configuration is a counterflow premixed flame between two opposing axisymmetric nozzles separated by a distance L, as shown in figure 1. The conservation equations for this configuration can be found in Refs.,[6,7] where a semi-compressible formulation was used in order to capture fast transients associated with gasdynamic compressibility effects.

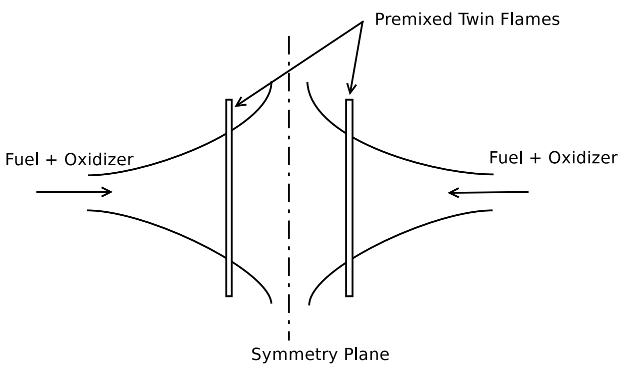

Figure 1. Counterflow premixed twin flame configuration.

The governing equations are solved using OPUS,[7] which is an opposed-flow solver using a one-dimensional similarity coordinate. The code employs variable-order implicit time integration with adaptive time stepping for robust handling of numerical stiffness.[8] The code is interfaced with CHEMKIN[9] and Transport[10] packages for computing detailed reaction rates and transport properties. A zonal grid refinement is used to obtain accurate solutions for the flame moving in space.

For the methane/air system considered in this study, the detailed chemical kinetic mechanism of GRI-Mech 2.11[11] has been used. A strained symmetric back-to-back premixed flame is established by supplying reactant mixture at identical conditions from both nozzles, such that only half of the domain is actually solved by the symmetry boundary condition.

In this finite-distance nozzle configuration, the inlet velocity is specified directly, but the corresponding strain rate is computed from the solved flow field *a posteriori*. A desired strain rate is thus obtained by trial and error for the inlet velocities. The strain rate is then held fixed by maintaining the inlet axial velocity for various inlet composition conditions. For all cases considered, the inlet temperature and pressure are set at 300 K and 1 atm, respectively. The spacing between the nozzles was fixed at 1 cm.

To study unsteady composition effects, the time-varying fuel concentration at the nozzle inlet is given by:

$$X_{\mathrm{CH_4}}(t) = X_{\mathrm{CH_4},0}[1 - A(1 - \cos(2\pi f t))] \quad (1)$$

where $X_{\mathrm{CH_4}}$ is the methane mole fraction, t is time, $X_{\mathrm{CH_4},0}$ is the initial value of the equivalence ratio, and A and f are the amplitude and frequency of equivalence ratio oscillation, respectively. At each instant, the loss or gain in methane composition is compensated by adding or removing an equivalent amount of air. For lean mixtures near extinction, which is the main interest of the present study, this is almost equivalent to fluctuating the equivalence ratio as:

$$\phi(t) = \phi_0[1 - A(1 - \cos(2\pi f t))] \quad (2)$$

where ϕ_0 is the initial equivalence ratio.

III. Flame Behavior

III.A. Steady Response

As a reference case, steady flame behavior is studied. In this case, at any fixed equivalence ratio, the inlet axial velocity is changed until the desired strain rate is obtained. The strain rate is defined as:

$$\kappa = \frac{1}{2r}\frac{\partial}{\partial r}(vr) \quad (3)$$

which is computed at the maximum heat release location. As reported in previous study[4] this definition of the strain rate has been found to be an appropriate representation of the characteristic flow time scale at the flame position. Although the actual strain rate changes slightly with equivalence ratio for a fixed inlet velocity, this variation is negligible and an approximate value is taken.

To obtain steady flammability limits at any fixed strain rate, the equivalence ratio is reduced until a steady flame no longer exists. This minimum equivalence ratio is defined as the steady flammability limit (ϕ_s), which is thus a function of strain rate, following our earlier study.[1] Three representative values of the strain rate were chosen, for which the maximum flame temperature is plotted against the equivalence ratio in figure 2. It is evident that the steady flammability limit increases with increasing strain rate. The specific values are found to be ϕ_s = 0.56, 0.65, and 0.71 for κ = 300 s^{-1}, 715 s^{-1} and 1070 s^{-1}, respectively. These three cases will be considered the baseline steady solutions in the next section.

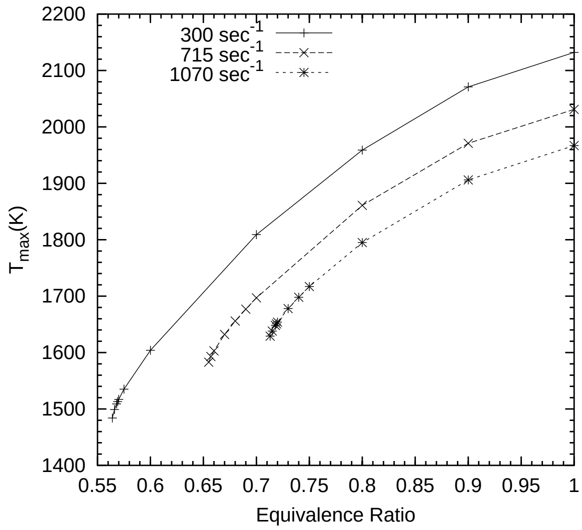

Figure 2. Flame temperature as a function of equivalence ratio at various strain rates.

III.B. Unsteady Response

Next, the response of flame to unsteady composition oscillation is studied. Mixture equivalence ratio is oscillated in the functional form given in equation 2. Typical limit-cycle flame response to the imposed sinusoidal variations in the equivalence ratio is shown in figures 3 and 4 for two different strain rates considered. In these figures, the maximum flame temperature is plotted against the instantaneous value of the equivalence ratio measured at the flame base, which is defined at the position where the temperature is 302 K. In prescribing the unsteady equivalence ratio oscillation, $\overline{\phi}$ - ϕ_s is fixed to 0.029, and the amplitude of oscillation is taken as the maximum without

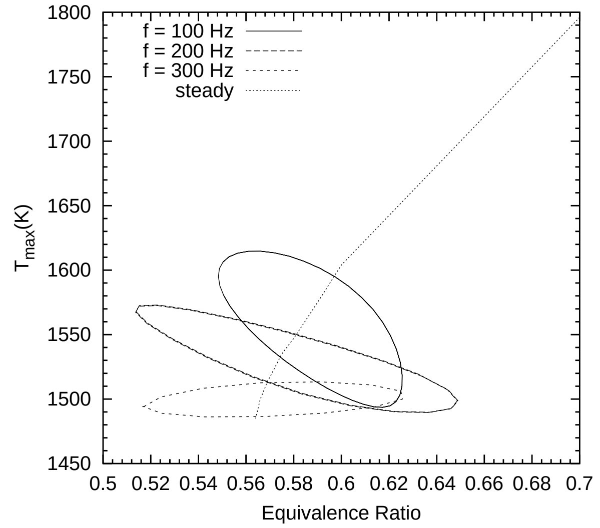

Figure 3. Flame temperature response to equivalence ratio oscillation measured at flame base for $\kappa = 300$ s^{-1}.

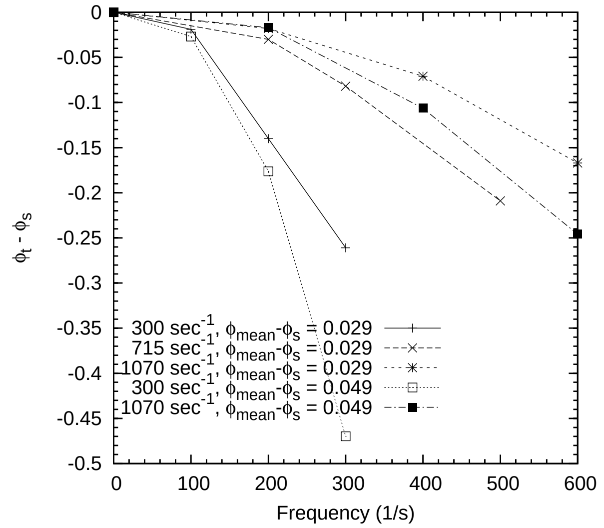

Figure 5. Difference between dynamic and steady flammability limits as a function of frequency for various strain rates and mean equivalence ratios.

leading to flame extinction. It can be seen that the flame response is considerably attenuated at higher frequencies, consistent with earlier studies.[1,2]

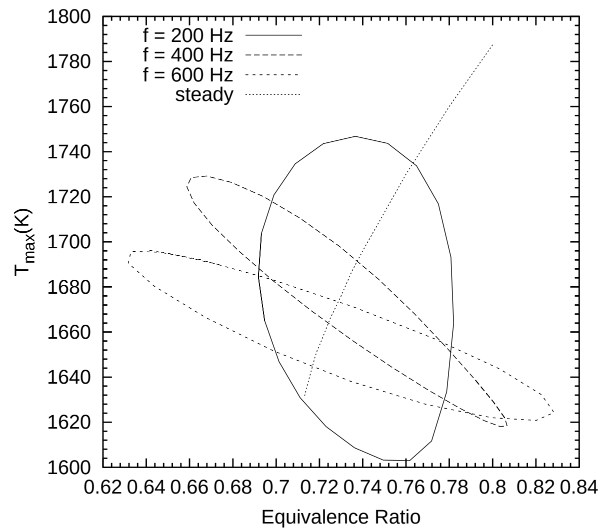

Figure 4. Flame temperature response to equivalence ratio oscillation measured at flame base for $\kappa = 1070$ s^{-1}.

It is also found that the flame sustains even when the instantaneous value of equivalence ratio drops much below the steady flammability limit, provided that the mean equivalence ratio is greater than the steady flammability limit. The minimum value of the equivalence ratio at the nozzle inlet is defined as the dynamic flammability limit (ϕ_t) for given frequency, mean equivalence ratio ($\overline{\phi}$) and strain rate (κ). The difference between dynamic and steady flammability limits as a function of frequency for various strain rates and mean equivalence ratios is shown in figure 5.

IV. Scaling Analysis

Similar to our previous study,[1] we now attempt to plot the dynamic flammability limit in terms of an appropriate nondimensional frequency parameter.

IV.A. Fixed Mean

We first fix the mean equivalence ratio for different strain rates and the unsteady flame response is examined. In particular, the mean equivalence ratio is fixed at 0.679 for two strain rates: $\kappa = 300$ sec^{-1} and 715 sec^{-1}. For each fixed strain rate, the amplitude of oscillation is increased until the flame reaches the extinction limit. Now, it is proposed in Sankaran and Im[1] that the dynamic flammability limit depends on strain rate, and mean and frequency of equivalence ratio oscillation. Since the mean is fixed, simple dimensional analysis gives only one scaling for the cut off frequency, which is $2\pi f/\kappa$.

In the figure 6, the difference between dynamic and steady flammability limits is plotted against this normalized scaling parameter for high and low strain rate cases. An excellent collapse of data is found for the two strain rate cases. Therefore, it can be concluded that the dynamic flammability limit is uniquely determined as a function of the frequency, strain rate and the mean equivalence ratio:

$$DFL = fn(f, \kappa, \overline{\phi}). \quad (4)$$

In Sankaran and Im,[1] it was found that above normalization of the unsteady frequency still left the dependence on the mean equivalence ratio, yielding an imperfect collapse of data (See figure 8 in Ref.[1]).

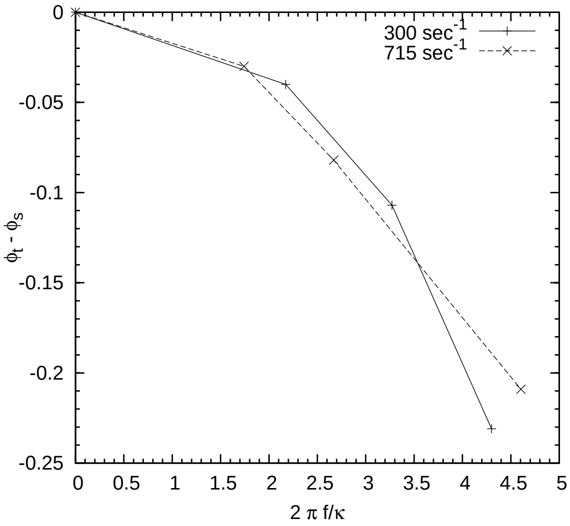

Figure 6. Difference between dynamic and steady flammability limits as a function of frequency scaled with flow strain rate alone. Mean equivalence ratio fixed to $\overline{\phi} = 0.679$, for both strain rates.

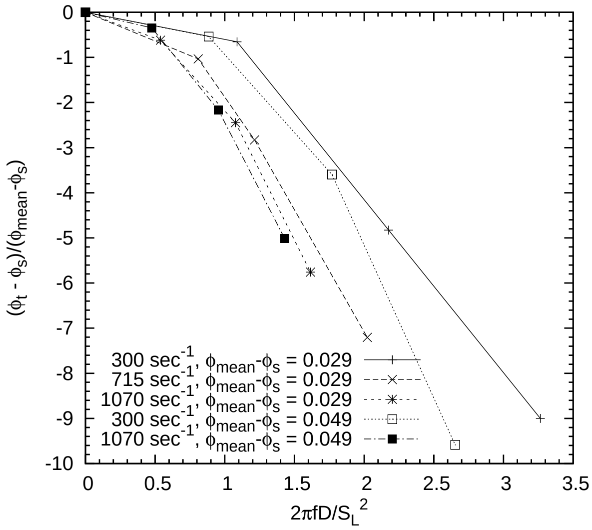

Figure 7. Normalized dynamic flammability limit extension as a function of frequency scaled with the nominal flame time.

This issue will be now thoroughly examined in the following subsection.

IV.B. Varying Mean

To assess the validity of the normalized frequency in more generalized conditions, the test is now extended by varying the mean equivalence ratio, $\overline{\phi}$. In the following discussion, the dynamic flammability limit extension (DFLE) is newly defined in a normalized form as

$$\mathrm{DFLE} = \frac{\phi_\mathrm{t} - \phi_\mathrm{s}}{\overline{\phi} - \phi_\mathrm{s}} \tag{5}$$

which is interpreted as the maximum instantaneous equivalence ratio drop with respect to the steady flammability limit, scaled in the unit of $\overline{\phi} - \phi_s$. The normalization is now needed in order to combine data sets for different mean equivalence ratio $\overline{\phi}$.

We first start with two existing methods to normalize the frequency and discuss their pitfalls. Subsequently, a new scaling parameter is proposed and the results are compared from the previous approaches.

It is conjectured that the normalized frequency proposed by Sankaran and Im,[1] $2\pi f/\kappa$, did not lead to a perfect collapse of data because the normalization does not properly account for the characteristic time scales of the flames subjected to different mean equivalence ratio. In other words, κ only represents the characteristic flow time scales, and no additional consideration is given to the variation in the flame time scale due to the mean equivalence ratio change.

In a related study, Lauvergne and Egolfopoulos[2] used a different form of frequency scaling in analogy with the Stokes second problem along with the assumption that the flame thickness scales as D/S_L, where D is the mass diffusivity of the reacting species and S_L is the laminar burning velocity. This has led to the nondimensional frequency in the form of $2\pi f D/{S_L}^2$. The results are plotted in figure 7, for various combinations of the strain rate and the mean equivalence ratio. Again, this alternative scaling did not successfully collapse the data. It is interesting to note that, in contrast to the normalization proposed by Sankaran and Im,[1] in this scaling S_L is mainly a function of the mean equivalence ratio and is insensitive to the strain rate. This is because, in lean methane-air mixtures, different contributions to the total preferential diffusion partly cancel and the effective Lewis number for the mixture becomes close to one, with regard to the mass burning rate.[5] Since the mixture behaves as nearly equi-diffusive with regard to the mass burning rate, the consumption speed is independent of strain rate.[3] To demonstrate this point, the laminar burning velocities were computed at various strain rates and equivalence ratios. Here the consumption speed,[13] S_c, has been adopted for comparison, which has been found to be a good measure of the upstream burning velocity.[12] In figure 8, the consumption speed for the methane-air flame is plotted as a function of the equivalence ratio for various strain rates. While the consumption speed varies widely over the range of the equivalence ratio, it is clearly seen that there is negligible dependence on the strain rate. This confirms that the frequency scaling proposed by Lauvergne and Egolfopoulos fails to account for the flow time scales associated with the strain rate.

Therefore, neither of the scalings discussed above

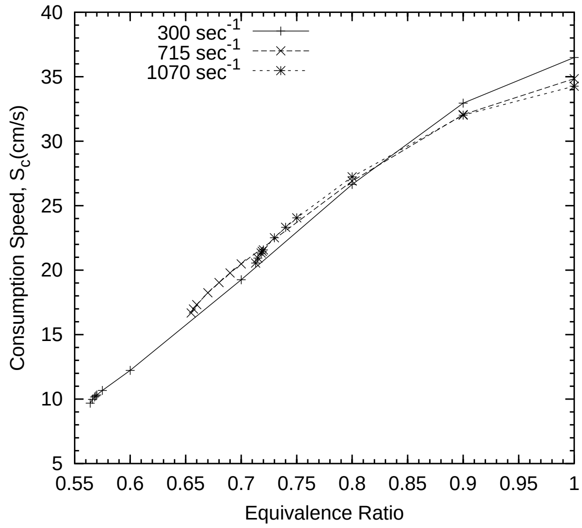

Figure 8. Consumption speed as a function of equivalence ratio for various flow strain rates.

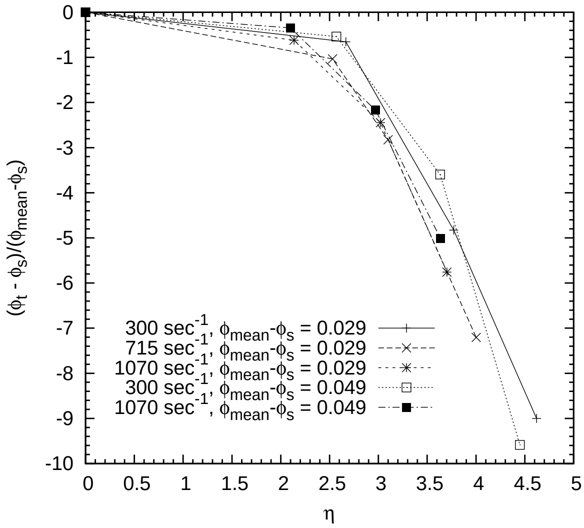

Figure 9. Normalized dynamic flammability limit extension as a function of the nondimensional frequency (η) defined in equation 6.

can successfully collapse the data over a range of strain rates and mean equivalence ratio. An alternative frequency scaling to incorporate both the flow and flame time scales is sought in the following.

In analogy with the Stokes' second problem as discussed in Ref.,[14] a nondimensional frequency is defined as

$$\eta = \delta\left(\frac{\omega}{2D}\right)^{1/2} \tag{6}$$

where ω is the angular frequency, $\omega = 2\pi f$, D is the mass diffusivity of methane into the bulk mixture, and δ is the flame thickness. Here we adopt the thermal flame thickness based on the temperature profile:

$$\delta = \frac{T_b - T_u}{(dT/dx)_{max}} \tag{7}$$

for which the steady solutions at the mean equivalence ratio are used.

The plot of normalized DFLE against the normalized frequency is shown in figure 9. It is seen that the data sets for various strain rates and mean equivalence ratios collapse very well. Note that the major difference in the new parameter compared to that used by Lauvergne and Egolfopoulos[2] is that we now use the actual flame thickness, δ, instead of the nominal flame thickness, D/S_L. Since the mixture behaves as nearly equi-diffusive with regard to the mass burning rate, the consumption speed is independent of strain rate as discussed before, whereas δ depends strongly on both strain rate and equivalence ratio. Figure 10 shows the variation in the thermal flame thickness as a function of the mixture equivalence ratio for various strain rate conditions under study. Not only is δ a strong function of the equivalence ratio, but it is also sensitive to the strain rate variations. Therefore, the new frequency scaling properly incorporate time scales associated with both flow (strain rate) and flame strength (equivalence ratio), leading to an improved collapse of data.

Compared to those proposed in previous studies, the main distinction of the new nondimensional frequency is the consideration of the *actual* measure of the transport time scale through the thermal flame thickness, which scales with δ^2/D. Based on this observation, an alternative scaling parameter is also suggested by directly computing the diffusion time scale, τ. Similar to the diffusion time scale defined by Lauvergne and Egolfopoulos,[2] the diffusion time scale is measured by the phase lag between the imposed equivalence ratio oscillation and the resulting flame temperature response. Figure 11 illustrates how the diffusion time is measured from the imposed and response oscillations. Based on this new parameter, the normalized DFLE is plotted against the nondimensional frequency, $\omega\tau$, as shown in figure 12. A good collapse of data comparable to the results in figure 9 is achieved. This further illustrates that the characteristic transport time scales in the flame are the key factor in determining the flame response to the unsteady fluctuations.

In summary, a generalized scaling of the unsteady flammability limit response to the imposed composition oscillation is obtained from the two alternative ways. Both definitions account for the actual transport time scales occurring in the flame thickness, thereby leading to much better collapse of the data compared to those proposed in previous studies. It is of interest to find that scaling of highly unsteady flame behavior can be done successfully by using the

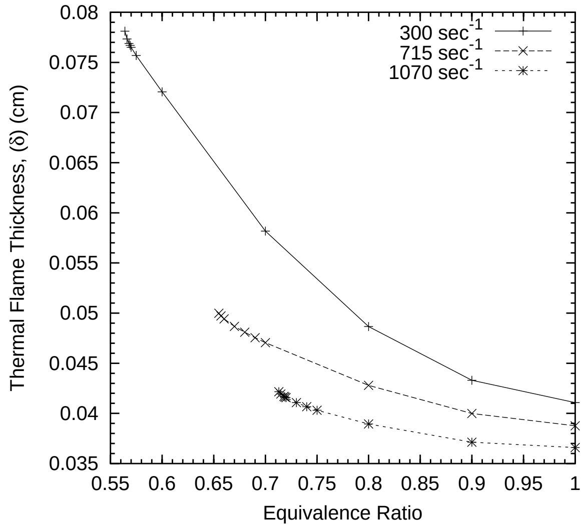

Figure 10. Thermal flame thickness, δ, as a function of the equivalence ratio for various strain rates.

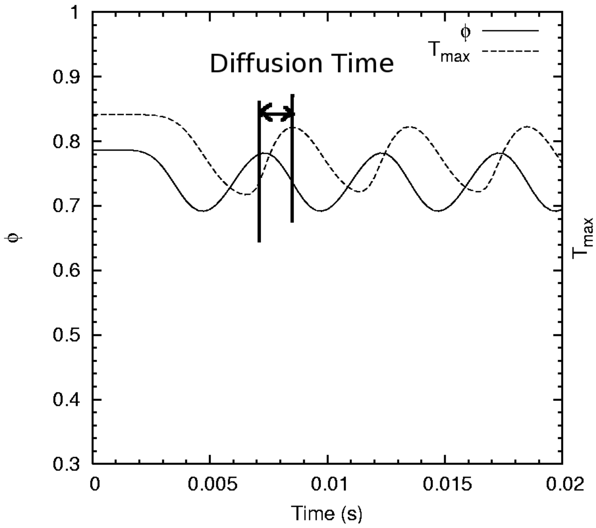

Figure 11. Diffusion time scale determined as the phase lag between the imposed equivalence ratio oscillation at the flame base and the flame temperature response.

flame parameters from steady solutions. This is attributed to the fact that flames behaves as a low-pass filter; any unsteady flucutations with characteristic time scales much shorter than the inherent flame time scales does not affect the flame response.

V. Universal Extinction Criterion

Consideration of a proper flame time scale is closely related to the determination of stretch-induced flame extinction. In a recent study by Cho *et al*,[15] a universal extinction criterion was proposed by properly defining the local Karlovitz number based on the actual flame thickness and speed. Specifically, the local Karlovitz number is defined based on the ratio of the local reaction time to the characteristic flow time:

$$Ka = \frac{\delta}{S_L}\kappa \tag{8}$$

where δ is the thermal flame thickness defined in equation 7, and S_L is the flame speed measured as the minumum flow speed upstream of the flame. For steady counterflow flames, Cho *et al* found that the local Karlovitz number at extinction was approximately 1.1, irrespective of the equivalence ratio. Here we attempt to apply the same concept to the unsteady flame phenomena.

For a typical unsteady flame near the extinction condition, the instantaneous local Karlovitz number was monitored in time and plotted in figure 13. It is clearly seen that local Karlovitz number in an unsteady flame also oscillates in response to the imposed fluctuations. In order to sustain combustion, it was found that the maximum instantaneous local Karlovitz number must not exceed a critical limit. In this case shown, this peak value of approximately 1.3 occurs at 0.022 sec. This maximum local Karlovitz number is monitored for a particular set of $\overline{\phi}$, κ, and f.

Figure 14 shows the maximum local Karlovitz number versus frequency for a range of mean equivalence ratio and strain rate conditions. It is seen that the local Karlovitz number based on actual flame thickness remains almost constant irrespective of strain rate, and mean and frequency of equivalence ratio oscillation. The value of this constant is found to be approximately 1.4. Therefore, the present work extends the observation by Cho *et al* to unsteady flame phenomena. This further attests to the conclusion that the key parameter to describe the criticality phenomena in steady and unsteady flames is the actual transport time scales.

VI. Conclusion

In this paper, the concept of dynamic flammability limits was further investigated and a universal scaling parameter was proposed to describe the flame behavior for a wide range of conditions. Starting from the observation that the dynamic flammability limit is a function of κ, f, and $\overline{\phi}$, a proper definition of nondimensional dynamic flammability limit extension was presented and several alternative scaling for the unsteady frequency were proposed. In contrast to previous studies, the two frequency scaling parameters were defined based on the actual flame thickness and diffusion time scales in order to better represent the characteristic transport time scale within the flame zone. It was demonstrated that the

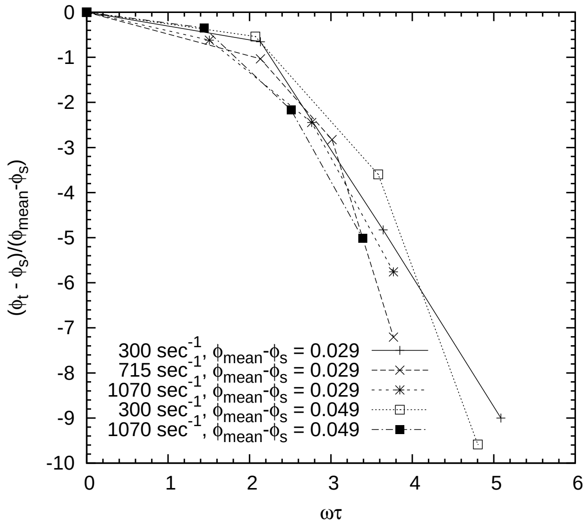

Figure 12. Normalized dynamic flammability limit extension as a function of a nondimensional frequency parameter based on the phase lag (τ)

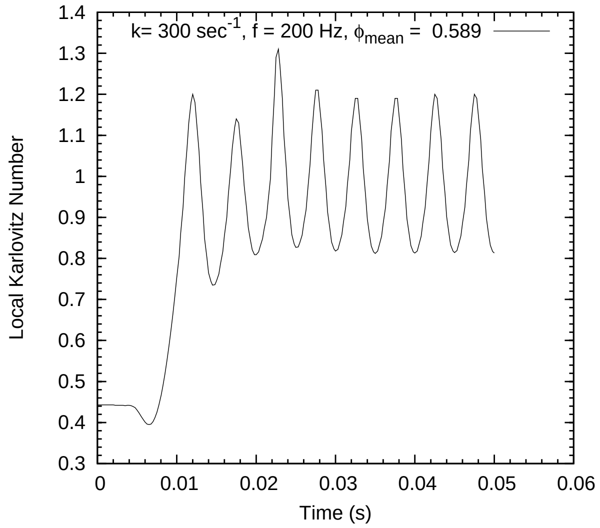

Figure 13. Local Karlovitz number as a function of time for a flame near the unsteady extinction limit: $\overline{\phi} = 0.589$, $f = 200$ s^{-1}.

new parameters successfully collapse the data for a wide range of strain rate and mean equivalence ratio. Therefore, the proposed scaling can be used as a universal criterion in predicting the unsteady flame extinction for a wide range of physical parameters.

As a related subject, a universal extinction criterion for the unsteady flame phenomena was also investigated based on local Karlovitz number. It was demonstrated that the maximum local Karlovitz number for unsteady flames near extinction remains reasonably constant, irrespective of strain rate, frequency, and mean of equivalence ratio oscillation. Therefore, the local Karlovitz number was found to be a universal measure of extinction conditions for both steady and unsteady strained flames.

Acknowledgments

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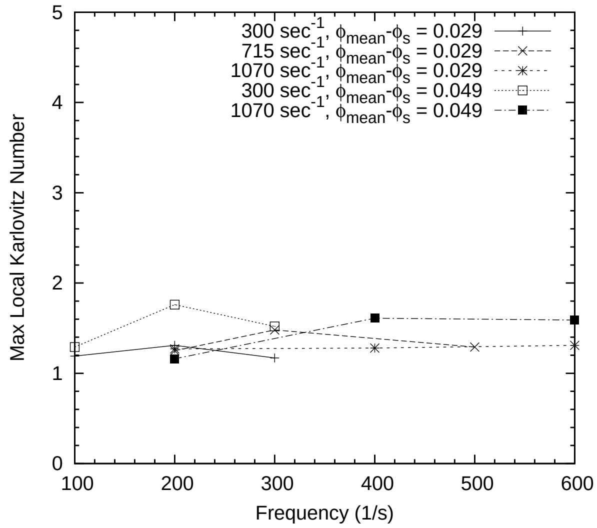

Figure 14. Maximum local Karlovitz number as a function of frequency for various strain rate and mean equivalence ratio conditions.

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