The existence of a critical dissipation rate, above which a nonpremixed flame is extinguished, has been known for decades. Recent advances in modeling have allowed the simulation of turbulent nonpremixed flames that include local extinction as a consequence of the stochastic variation in mixing rates. In this paper we present the critical dissipation impulse magnitude that will lead to extinction even if the mean dissipation rate is well below the criteria for a steady flame. This critical impulse magnitude depends on the time-integrated excess dissipation rate, stoichiometric factors and the form of the S-curve describing the steady-state flame. This criteria is evaluated in a diverse set of flames including n-heptane, diluted n-heptane and CO/H₂/N₂ mixtures.

1 Introduction

A criteria for which turbulent flames are extinguished is key to predicting such diverse phenomena as fire suppression and flame stabilization. While the theoretical basis for extinction of an individual laminar nonpremixed flamelet (here used broadly to indicate a stoichiometric fluid element where chemical reactions take place due to molecular mixing as opposed to the turbulent flame which is a collection of flamelets) has been known for decades [1], the details of extinction in turbulent flames have been coming to light more recently as stochastic simulations of localized extinction and reignition are conducted [2–4]. The present paper is a step toward quantifying the frequency of turbulent flamelet extinction without the need to carry out a stochastic simulation. To accomplish this, a criteria for extinction due to an unsteady variation in the mixing rate first proposed in [2] is evaluated.

For an individual nonpremixed flamelet, extinction may occur if the rate of heat loss exceeds the rate of chemical heat release. This rate of heat loss can be characterized by the scalar dissipation rate, \( \chi \), defined in terms of the gradient of the mixture fraction, \( Z \), as \( \chi = 2D|\nabla Z|^2 \). All dissipation rates in this paper are evaluated at the stoichiometric point. The response of a flamelet to a steady dissipation rate can be characterized using the well-known S-curve showing the maximum temperature as a function of dissipation rate. The upper and middle branches are shown in Fig. 1 for boundary conditions considered in this work. The upper branch represents stably burning flames while the middle branch is unstable; flames will tend to move away from the middle branch toward the upper or lower branches. Note that the S-curve abscissa in this paper is \( \chi \) rather than the Damköhler number, which is inversely proportional to \( \chi \); using \( \chi \) along the abscissa allows easier interpretations of changes in the mixing rate, but results in a reversed S-curve. Above a critical
dissipation rate, heat losses exceed heat-release rates and a steady flame cannot exist; this point, \( \chi_q \), is associated with extinction for steady flames.

One problem that arises in the application of the S-curve describing steady flamelets is that the instantaneous value of \( \chi \) varies with time in turbulent flows about whatever effective mean value is determined by the large-scale mixing. The distribution of \( \chi \) can be approximated as log normal, and for moderate to large Reynolds numbers \( \chi \) may vary over several orders of magnitude. In direct numerical simulations, the local dissipation rate has been shown to vary over time scales comparable to the Kolmogorov time scale [5], so that large fluctuations in \( \chi \) may occur over short periods of time. The present paper addresses how the magnitude and time scale of rapid fluctuations in \( \chi \) determine whether or not extinction will occur.

A number of studies addressing the response of individual flames to unsteady mixing time scales have identified the fact that flames are more resistant to extinction for high frequency or short period mixing rate fluctuations. Ghoniem et al. [6] showed that by increasing the frequency one can go to higher amplitude fluctuations before the flame is extinguished. Mauss et al. [7] showed that, for a fixed peak dissipation rate, exceeding \( \chi_q \) for a longer duration required a greater subsequent reduction in the dissipation rate to prevent extinction. These two observations can be coupled together in an extinction criteria first proposed in [2] and described in the subsequent section.

2 Method and Approach to Analyzing Results

For ease in interpretation of the results and to simplify the form of the equations, a simplified version of the flamelet equations written in the mixture fraction coordinate is employed. While detailed chemical kinetics and thermo chemistry (i.e. enthalpies) are retained, all transport properties
are assumed identical so that Lewis numbers are unity, and the species diffusion is presumed to follow Fick’s Law so that the effect of gradients in the molecular weight on diffusion are ignored. Simplified species and energy equations are

\[
\frac{dY_i}{dt} = \frac{\chi}{2} \frac{d^2Y_i}{dZ^2} + \frac{\omega_i}{\rho} \tag{1}
\]

\[
\frac{dT}{dt} = \frac{\chi}{2} \frac{d^2T}{dZ^2} - \frac{\chi}{2} \sum_i \left(1 - \frac{c_{p,i}}{c_p} \right) \frac{dY_i}{dZ} \frac{dT}{dZ} - \sum_i \frac{\omega_i h_i}{\rho c_p} \tag{2}
\]

Here \(Y_i, \omega_i, c_{p,i}\) and \(h_i\) are the mass fraction, production rate, specific heat and enthalpy, respectively, of species \(i\); \(\rho\) and \(c_p\) are the mixture density and specific heats. The scalar dissipation rate, \(\chi\) is allowed to vary in the mixture fraction coordinate with the standard counterflow configuration form, \(\chi(Z) = \chi_0 \exp(-2 \text{erfc}^{-1}(2Z)^2)\). These equations are evolved forward in time from a steady-state initial condition using the FlameMaster code [8]. During the temporal evolution the value of \(\chi_0\) is varied so that the stoichiometric dissipation rate follows either a square-shaped, triangle-shaped or sinusoidal impulse with an initial magnitude \(\chi_1\) and a peak value of \(\chi_2\) as indicated in Fig. 2. In order to determine \(\chi_q\), to define the shape of the S-curves in Fig. 1 and to generate initial conditions for the transient flames, a series of steady flamelets are also computed using continuation methods.

Computations are conducted using varied fuel mixtures to provide a wide range of parameter space. Fuel mixtures employed are pure n-heptane, n-heptane diluted with nitrogen (50% by mass) and a CO/H\(_2\)/N\(_2\) mixture (55.4%/3%/41.6% by mass). The chemical-kinetic mechanisms employed are available from the author and are similar to those described in [9, 10]. The present results are insensitive to the mechanism.

Unsteady extinction results can be explained in terms of the S-curve [7]. Variations in \(\chi\) tend to move the state away from the S-curve as depicted with dotted arrows in Fig. 3. An increase in the
Figure 3: Possible trajectories for unsteady flamelets shown relative to the steady state by dotted arrows.

dissipation rate above $\chi_q$ will result in the flame temperature dropping with time (segments 1 and 2 in Fig. 3). If the duration for which $\chi > \chi_q$ is sufficiently short, the subsequent reduction in the dissipation rate leads to a flame state in between the upper and middle branches of the S-curve and the flame, given sufficient time, returns to the steady state value on the upper branch (segments 3 and 4 in Fig. 3). Conversely, if the duration for which $\chi > \chi_q$ is sufficiently long, a reduction in the dissipation rate will lead to a flame state below the middle branch, in which case the flame temperature will continue to drop (segments 5 and 6 in Fig. 3). Though it is beyond the scope of the present work, we note in passing that the steady-state middle branch only represents an approximate dividing line because, particularly with detailed chemistry, the transient flame state differs from that at steady-state.

In Ref. [2] a criteria was proposed for extinction when fluctuations in the dissipation rate exceed $\chi_q$ for a period in the course of turbulent flame evolution. This criteria is based on estimates for the heat-release rate and heat-dissipation rate. The maximum heat-release rate can be approximated by the steady mixing rate at the quenching condition, equating the second and fourth terms in the energy equation in Eq. 2

$$\left( \sum_i \frac{\omega_i h_i}{\rho c_p} \right)_{max} \approx -\frac{\chi_q}{2} \frac{dT}{dZ^2}. \quad (3)$$

It is presumed that while $\chi_q$ is exceeded, but while the temperature is still above the middle branch, heat release may continue at approximately this rate. The diffusive term can be estimated as $-\chi T Z_{st}^{-2} (1 - Z_{st})^{-2}$ so that, for $\chi > \chi_q$ and temperatures above the middle branch, the rate of change in the thermochemical state, represented by temperature, can be estimated (neglecting the enthalpy flux for simplicity) as

$$\frac{dT}{dt} = \chi \frac{d^2T}{2 dZ^2} - \left( \sum_i \frac{\omega_i h_i}{\rho c_p} \right)_{max} \approx -\frac{(\chi_q - \chi)}{2} \frac{d^2T}{dZ^2} \approx \frac{(\chi_q - \chi) T}{Z_{st}^2 (1 - Z_{st})^2}. \quad (4)$$
This creates a plausible time scale for extinction. The time scale, the inverse of the right-hand side of Eq. 4, is the exponential decay constant since the solution of Eq. 4 is of the form

$$\frac{T_2 - T_0}{T_1 - T_0} = \exp(-A\Xi)$$

(5)

where

$$\Xi = \frac{\int_{\chi > \chi_q} (\chi - \chi_q) dt}{Z_{st}^2 (1 - Z_{st})^2}.$$  

(6)

Here $A$ is a proportionality constant since Eq. 4 is only an approximate equality. A better approximation would involve a prediction of the reaction zone thickness as can be obtained through asymptotic means, for example [1, 11]. Here $T_0$ is the temperatures of the reactants, $T_1$ the steady flame temperature before the scalar dissipation rate rises and $T_2$ the predicted unsteady flame temperature after $\chi$ is again less than $\chi_q$. In the numerator of $\Xi$ the integral $\int_{\chi > \chi_q} (\chi - \chi_q) dt$ appears. This is the integral over time of the excess dissipation above $\chi_q$ as indicated by the hatched region in Fig. 2. If the value of $T_2$ predicted by Eq. 6 when $\chi$ returns to its original value, $\chi_1$, is below the middle branch, then we expect the flame to be extinguished.

3 Results and Discussion

In order to evaluate Eq. 6 as an unsteady extinction criteria, unsteady simulations were performed as described in the previous section. Using a bisection search algorithm, the critical value of $\Xi$ that delineates the division between extinguished and non-extinguished flames, $\Xi_q$, is identified as a function of the initial dissipation rate, $\chi_1$, and the maximum dissipation rate, $\chi_2$, for the three profiles indicated in Fig. 2 by varying the duration of the pulse. As an example of the evolution of the thermochemical state, Fig. 4 shows the temperature and dissipation rate as a function of time along with the temperature-dissipation phase plot for three pairs of simulations with durations characterized by $\Xi$ somewhat above (dashed lines) and below $\Xi_q$ (solid lines). It is noted that a square temporal profile for $\chi$ results in virtually no change in temperature between $\chi_1$ and $\chi_2$ and the solution moves well away from the stable S-curve solution (the duration of the transition is 1% of the total impulse period). For a triangle (or sinusoidal) temporal profile, however, the magnitude and period of the pulse determine whether or not the temperature follows the S-curve. For $\chi_2/\chi_q$ not very large, the duration of the impulse for $\Xi$ near $\Xi_q$ is long and the gradual changes in $\chi$ allow the transient state to largely follow the S-curve (i.e. the middle panes of Fig. 4). For larger $\chi_2/\chi_q$ (lower panes of Fig. 4) the solution increasingly moves away from the S-curve.
Figure 4: The temporal evolution of $\chi$ and the temperature (left) and the temperature-dissipation phase plot (right) for one square and two triangle-shaped dissipation impulses.
The value of $\Xi_q$ is determined to within 1% for a wide range of $\chi_1/\chi_q < 1$, $\chi_2/\chi_q > 1$ and for the three fuel mixtures indicated. These are plotted in Fig. 5, and a number of observation can be made. For smaller $\chi_1/\chi_q$ where the required reduction in the temperature to cross the middle branch of the S-curve is greater, the magnitude of $\Xi_q$ is generally greater as predicted by Eq. 6.

For sinusoidal and triangle-shaped impulses, as $\chi_2/\chi_q$ approaches unity the magnitude of $\Xi_q$ approaches the value for a flame near extinction ($\chi_1/\chi_q \rightarrow 1$). This occurs because the flame has time to adapt to the near-extinction state as indicated in the middle panes of Fig. 4. Because the change in $\chi$ is rapid for square impulses, this is not observed in those curves. To quantify the meaning of rapid versus gradual changes in the dissipation rate, one must compare $dT/dt$ from Eq. 4 with $(dT/d\chi)(d\chi/dt)$. If the latter is small relative to the former, then the flame state will follow the S-curve, until such a condition is violated (as when $dT/d\chi \rightarrow -\infty$ at $\chi_q$). As a preliminary estimate of the significance of rapid fluctuations, we note that Yeung and coworkers [5, 12] looked at the dynamics of flame surface straining using direct numerical simulations. They observed that the integral time scales for variation in strain rates are only somewhat larger than the Kolmogorov time scale; in Ref. [5] they indicate this is three times the Kolmogorov scale. Therefore, we expect rapid fluctuations in the dissipation rate are typical in large Reynolds number turbulence.

For rapid changes in $\chi$, as occurs for large $\chi_2/\chi_q$ and for square profiles, the value of $\Xi_q$ becomes independent of the shape of the impulse and depends on the initial conditions. In this case, we identify the magnitude of $T_1$ and $T_2$ appearing in Eq. 6 by reading from the appropriate S-curve in Fig. 1 at the location $\chi_1$ and normalize $\Xi_q$ by $\ln(T_2 - T_0)/(T_1 - T_0)$ giving the constant of proportionality, $A$, in Eq. 6. This is plotted in Fig. 6. It is observed in Fig. 6 that for large $\chi_2/\chi_q$ the curves come together (for small $\chi_2/\chi_q$ the change in $\chi$ is gradual so that $T_1$ should be taken near extinction resulting in the convergence evident in Fig. 5) indicating that the relationship in Eq. 6 is a suitable predictor of unsteady extinction criteria for large fluctuations in the dissipation rate.

There is still some systematic variation in the value of $A$ indicated in Fig. 6. In particular, as $\chi_1/\chi_q \rightarrow 1$, the appropriate magnitude of $A$ is larger. While space limitations prevent a graphical demonstration, this occurs because the reaction rates are initially higher in flames with initially high dissipation rates. The reaction rates are observed to transiently exceed the reaction rates at $\chi_q$ leading to greater resistance to extinction than predicted in Eq. 6. This is a purely transient phenomena occurring as the temperature remains above the steady-state temperature at $\chi_q$ (so that the kinetic rates are still fast) and the high dissipation rates mix reactants more rapidly. This phenomena will require further investigation.
Figure 5: The critical value of $\Xi$ corresponding to extinction for various dissipation impulses. Solid lines are sinusoidal, dashed lines are square-shaped and dash-dot lines are triangle-shaped profiles.
Figure 6: $\Xi_q$ normalized by $\ln(T_2 - T_0)/(T_1 - T_0)$ giving the constant of proportionality, $A$ in Eq. 6. Solid lines are sinusoidal, dashed lines are square-shaped and dash-dot lines are triangle-shaped profiles.
4 Conclusion

A criteria indicating the magnitude of a scalar-dissipation impulse leading to extinction has been investigated. The quantity $\Xi$, involving the time-integrated excess dissipation over $\chi_q$ and appropriate stoichiometric factors, has been shown to provide a sufficient description of the heat losses during a brief period where the dissipation reaches values much greater than $\chi_q$ so that, when coupled with knowledge of the S-curve temperature-dissipation relationship, extinction can be reasonably well predicted. When the rate of change in dissipation is fast relative to the rate of response of the temperature to changes in $\chi$, this criteria is independent of the profile of the dissipation impulse, but does depend on the temperatures at the steady-state condition along the S-curve prior to the impulse. When the dissipation rate changes gradually, the criteria is independent of the initial steady-state conditions, but depends on the state along the S-curve near extinction or wherever the rate of change in the dissipation rate becomes large. For initial and or maximum dissipation rates near $\chi_q$, this criteria based on $\Xi$ slightly over predicts heat losses, and would thus predict extinction too soon if not corrected. A further study with greater detail is available separately [13].
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