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Stochastic modeling of unsteady extinction in turbulent non-premixed combustion

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Abstract

Turbulent fluctuations of the scalar dissipation rate have a major impact on extinction in non-premixed combustion. Recently, an unsteady extinction criterion has been developed (Hewson, 2013) that predicts extinction dependent on the duration and the magnitude of dissipation rate fluctuations exceeding a critical quenching value; this quantity is referred to as the dissipation impulse. The magnitude of the dissipation impulse corresponding to unsteady extinction is related to the difficulty with which a flamelet is exintguished, based on the steady-state S-curve.

In this paper we evaluate this new extinction criterion for more realistic dissipation rates by evolving a stochastic Ornstein–Uhlenbeck process for the dissipation rate. A comparison between unsteady flamelet evolution using this dissipation rate and the extinction criterion exhibit good agreement. The rate of predicted extinction is examined over a range of Damköhler and Reynolds numbers and over a range of the extinction difficulty. The results suggest that the rate of extinction is proportional to the average dissipation rate and the area under the dissipation rate probability density function exceeding the steady-state quenching value. It is also inversely related to the actual probability that this steady-state quenching dissipation rate is observed and the difficulty of extinction associated with the distance between the upper and middle branches of the S-curve.

Keywords: Extinction; Unsteady flames; Non-premixed flame; Scalar dissipation rate; Turbulence

1. Introduction

To minimize pollutant formation and maximize volumetric combustion efficiency, it is desirable to maximize the rate of combustion subject to the limits of overall flame stability. These limits of

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flame stability are determined by the rate of local extinction.

Steady-state flame extinction in non-premixed combustion occurs when a mixing rate, here expressed as the scalar dissipation rate, χ, exceeds some critical value, χ_q, that depends on the chemical rates. Here and throughout this paper, except the flamelet equations(9) and (10), χ refers to the value at the stoichiometric location, Z_{st}. For $\chi > \chi_q$ no steady-state flame exists, although under unsteady mixing rates brief transients above the critical value can occur without extinguishing the flame [2,3]. Recently, an unsteady extinction criterion has been developed that predicts extinction dependent on the duration and magnitude of dissipation-rate excursions where $\chi > \chi_q$ and the shape of the S-curve, the locus of maximum flame temperatures as a function of χ for steady-state solutions [1]. This new extinction criterion is related to a dissipation impulse, the time-integrated excess mixing rate, where $\chi > \chi_q$, that impulsively cools the flame. Unfortunately, the statistics of this dissipation impulse, referred to as Ξ below, have not previously been investigated. In the present work we investigate these statistics using one of the simplest possible models for the dissipation evolution in turbulent flows, an Ornstein–Uhlenbeck (OU) process for the logarithm of the dissipation rate. The OU process approach for dissipation rate modeling was first developed by Pope and Chen [4], and here this same model is applied to the scalar dissipation rate. It has been used to investigate the influence of stochastic fluctuations of the scalar dissipation rate on the solution of the flamelet equations [5] as well as on local extinction and re-ignition in flamelet modelling of non-premixed turbulent combustion [6].

The extinction process for turbulent non-premixed flames has been studied with direct-numerical simulations (DNS) using one-step chemistry [7], reduced chemistry [8] and detailed chemistry [9,10]. Significant insights into unsteady extinction also come from stochastic one-dimensional turbulence (ODT) simulations where it was observed that the probability of observing local extinction was significantly greater than the probability that $\chi > \chi_q$ suggesting a time-scale separation where local extinction was rapid relative to the global evolution of the probability of extinction [11]. Further insight came from DNS over a range of Reynolds numbers where the change in variance for the dissipation rate affects the statistics of very large χ [12]. Pdf evolution approaches to modeling turbulent combustion have a stochastic approach and also contribute to the prediction of extinction in turbulent flames [13].

In the present work, the extinction criterion is evaluated for scalar dissipation rate fluctuations that are generated by a stochastic Ornstein-Ulenbeck process. In the following sections, the governing equations are first stated and discussed. Finally, the results for the extinction criterion in comparison to unsteady flamelet simulations are presented and the rate of extinction for different Damköhler and Reynolds numbers is examined.

2. Model formulation

2.1. The dissipation impulse

A quantitative model of unsteady flamelet extinction was recently derived based on a simplified energy equation in terms of an integrated excess dissipation rate over a continuous period where $\chi > \chi_q$ [1]. This integrated quantity is referred to as the dissipation impulse. Here we just present the final results and refer to [1] for a full derivation with explanations. Starting from the simplest form of the energy equation and using approximations for the reaction rate and the diffusive term, we end up with a formulation that describes the peak flame temperature as a function of χ during periods where $\chi > \chi_q$. The integral of that expression yields

$$\frac{T_2 - T_\infty}{T_1 - T_\infty} = \exp(-\Xi), \qquad (1)$$

where

$$\Xi = \frac{A \int_{\chi > \chi_q} (\chi(t) - \chi_q) \mathrm{d}t}{2 Z_{st}(1 - Z_{st})\epsilon}. \qquad (2)$$

Here Z_{st} is the stoichiometric mixture fraction, ϵ is a reaction zone thickness related to Z_{st}, A is a constant equal to 0.5, T_1 is the initial flame temperature, T_∞ is the ambient temperature and T_2 is the predicted flame temperature at time when $\chi(t)$ returns to the initial χ below χ_q. Ξ defined in Eq. (2) describes the dissipation impulse causing a temperature drop during $\chi(t) > \chi_q$. Figure 1 graphically illustrates the integral in Eq. (2). If $T_2 < T_m$, where T_m is the middle branch temperature at $\chi = \chi_1$, the flame will extinguish as discussed in Hewson [1]. The critical value where $T_2 < T_m$ is denoted Ξ_q and depends only on the shape of the steady-state S-curve. Values of Ξ_q depend on the typical dissipation rate and range from 0.8 to 0.3 with smaller values corresponding to the typical state being closer to extinction [1]. This is because if χ approaches χ_q the temperature of the burning flame gets smaller and the corresponding

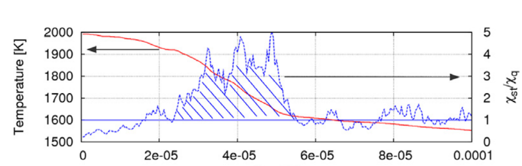

Fig. 1. Temporal evolution of $\chi(t)$ and $T_f(t)$ in an unsteady flamelet simulation following Eqs. (7) and (10). The horizontal line indicates $\chi_{st}/\chi_q = 1$ and the shaded area above the line represents the integral within Eq. (2).