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Flame index and its statistical properties measured to understand partially premixed turbulent combustion

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ABSTRACT

This work addresses some fundamental questions in the area of partially premixed combustion—what parameters control the fraction of flamelets that are premixed (versus non-premixed), and what are the locations of high probability of premixed (versus non-premixed) combustion? To answer these questions there is a need to measure the flame index (ξ) and its statistical properties, and this information previously has not been available. Flame index is $+1$ where a premixed flamelet exists and is -1 at the location of a non-premixed flamelet. A new method to measure flame index was developed that adds NO_2 to the air; acetone is used as one component of the fuel. Laser-induced fluorescence images indicate the locations of flamelets and whether the gradients of the fuel and O_2 are in the same direction or not. Flame index was measured in a gas turbine model combustor that was designed at DLR that is a good example of partially premixed combustion.

Measurements show how the mean flame index varies in space; near the fuel injector the combustion is 50% non-premixed and 50% premixed while downstream the flamelets are mostly premixed. This trend is consistent with two numerical simulations of swirl flames; however for simple lifted jet flames the premixed flamelets do not extend so far downstream. It was found that one parameter that controls the fraction of flamelets that are premixed is the ratio of the fuel injection velocity to the air velocity. Increasing this ratio increases the fraction of flamelets that are premixed because it increases the distance that the fuel stream penetrates into the more intense mixing region. Good signal-to-noise ratios of 24 (for acetone) and 13 (for NO_2) were achieved and an uncertainty analysis is presented that is based on calibration experiments.

1. Introduction

Recently there has been a considerable amount of interest in the area of partially premixed turbulent combustion. The term *partially premixed* indicates that premixed flames occur at some times at a point while non-premixed flames exist at other times at that same point. Partially premixed combustion should not be confused with *stratified premixed* combustion; the latter occurs when the fuel–air mixture ratio is not uniform in space but it always remains within the flammability limits so that none of the flamelets are non-premixed. One example of partial premixing is the base region of a lifted (initially non-premixed) jet flame [1–6]. Mixing occurs in the liftoff region and mixing may by assisted by adding co-flow air, cross-flow air, or swirling air [7–9]. A large number of practical devices burn fuel in the partially premixed mode since the reaction zone usually is lifted from the fuel injectors that are used in automotive, gas turbine, and rocket engines.

Important questions about partially premixed combustion are: what fraction of the flamelets are premixed, what controls this fraction, and what are the locations where there is a high probability of premixed flamelets? For example, near the base of a lifted jet flame the Direct Numerical Simulation (DNS) of Mizobuchi et al. [2] identified many regions of premixed combustion while at downstream locations the combustion was mostly non-premixed. They argued that premixed combustion is caused by the fuel–air mixing that occurs in the shear layers within the liftoff region. Cai et al. [10] explain that another example of partially premixed combustion is the upstream region of Sandia jet flame D [10] that is surrounded by a premixed pilot flame. A typical gas turbine combustor normally contains a relatively short, compact, and lifted flame that is expected to have regions that are partially premixed.

To understand and to model partially premixed combustion, a useful parameter is the Takeno flame index (ξ). It was defined by

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Yamashita et al. [1] to be the normalized dot product of the gradients of the fuel and oxidizer mass fractions (Y_F, Y_O):

$$\xi = \frac{\nabla Y_{F,\max} \cdot \nabla Y_{O,\max}}{\left|\nabla Y_{F,\max} \cdot \nabla Y_{O,\max}\right|}. \quad (1)$$

Consider the direction that is normal to a thin, wrinkled flamelet. The gradient in the fuel mass fraction is approximately a Gaussian-shaped function and its maximum value ($\nabla Y_{F,\max}$) occurs approximately in the middle of the layer. The denominator in Eq. (1) is the absolute value of the scalar dot product. For the premixed case the fuel and oxidizer gradients are aligned so the flame index is $+1$. For the non-premixed case the flame index is -1 if there is fuel on one side and air on the other side of the flamelet. If no flamelet exists at a location then the flame index at that location is defined as zero. As an example, suppose that there is a measurement error that causes the numerator of Eq. (1) to be 20% larger than the actual instantaneous value. This should not change the value of the flame index because the denominator always is the magnitude of the numerator. Thus the flame index only can take on values of $+1$ or -1 if a flamelet is present. An error in the instantaneous value of flame index occurs if the measurement error is so large that it causes the measured sign of ξ to be opposite to the actual sign. This occurs infrequently, as discussed in the uncertainty analysis presented below.

The global fraction of flamelets that are premixed (β) is defined to be:

$$\beta = \left\langle \frac{C}{A+C} \right\rangle, \quad (2)$$

where A and C are components of the probability density function (PDF) $Pr(\xi)$ of the flame index, and the brackets imply that spatial averaging is done over the entire flame. $Pr(\xi)$ consists of three delta functions located at $\xi = +1, -1$, and 0, so:

$$Pr(\xi) = A\delta(\xi+1) + B\delta(\xi) + C\delta(\xi-1), \quad (3)$$

where δ is the Dirac delta function. A is the probability of the occurrence of non-premixed flamelets since if $\xi = -1$ the first term in Eq. (3) becomes $A\delta(0)$, and the integral of $A\delta(0)\mathrm{d}\xi$ is A. B is the probability of no flamelet, and C is the probability of premixed flamelets. The mean flame index, $\overline{\xi}$, is the integral of $\xi Pr(\xi)\mathrm{d}\xi$ over all values of ξ, which is $(C-A)$. The sum $(A+C)$ is the probability that flamelets occur, so the probability that a flamelet is premixed is $C/(A+C)$.

Previous studies that have reported values of flame index have been limited to direct numerical simulations (DNS) and large eddy simulations (LES). DNS of Mizobuchi et al. [2] and Domingo et al. [5] showed that the base of a lifted jet flame contains many cusp-shaped regions and each region has a value of ξ that is either $+1$ or -1. A similar DNS result was reported for a lifted jet flame in a cross-flow by Grout et al. [8]. Luo et al. [9] described DNS computations of ξ when swirl was added to the flow. These DNS results indicate that the lifted base region has both premixed and non-premixed structures, as does a *triple-flame* [11,12].

To simulate partially premixed combustion at higher Reynolds numbers than can be achieved with DNS it becomes necessary to use Large Eddy Simulation (LES). With some LES submodels the probability density function of flame index $Pr(\xi)$ is determined first. Then different submodels are applied for premixed and non-premixed combustion, as described by Bray et al. [13], Domingo et al. [14], Knudsen and Pitsch [15,16], and Patel and Menon [17]. For example, the mean volumetric reaction rate of hydrogen (H_2) in a computational cell can be set equal to:

$$\overline{\omega_{H_2}} = \int_{-\infty}^{+\infty} \omega_{H_2} Pr(\xi)\mathrm{d}\xi = A\omega_{H_2,\mathrm{nonpre}} + C\omega_{H_2,\mathrm{pre}}, \quad (4)$$

where A and C are components of the PDF of flame index that is defined in Eq. (3). A premixed combustion submodel simulates the premixed reaction rate $\omega_{H_2,\mathrm{pre}}$ while a non-premixed combustion submodel simulates $\omega_{H_2,\mathrm{nonpre}}$. The proposed subgrid models [13–16] for the probabilities A and C are similar to subgrid models of scalar dissipation rate. The resolved-scale scalar gradient is first computed from values determined on the grid points and the model assumes that the sub-grid scalar gradient is proportional to this resolved-scale gradient. For example, Domingo et al. [14] assumes that the mean flame index in a cell of size Δ is:

$$\overline{\xi} = \mathfrak{F}_Z\chi_Z + \mathfrak{F}_c\chi_c. \quad (5)$$

The subgrid scalar dissipation rate, χ_Z, is modeled in the standard manner to be $\Delta^2\left|\widehat{\nabla Z}\right|^2/\tau$, where Δ is the cell size, $\left|\widehat{\nabla Z}\right|$ is the magnitude of the resolved-scale mixture fraction gradient, and τ is a time constant. Ref. [14] provides relations for the weighting functions $\mathfrak{F}_Z$ and $\mathfrak{F}_c$, the reactedness dissipation rate χ_c, and the time constant τ. Knudsen and Pitsch [16] propose a similar model; they also relate flame index to the gradients in mixture fraction and reactedness but in a different way than Domingo et al. [14]. A different LES approach is the progress variable (PV) method of Pierce and Moin [18], Ihme and See [19], and Ihme and Pitsch [20]. A flamelet library is generated by solving the flamelet equation for two independent variables (mixture fraction and progress variable). A number of other related simulations also have been reported [21–25]. There have been no assessments of the various sub-models due to the lack of measurements of the flame index.

While no measurements of flame index previously have been reported, numerous experimental studies have added acetone (CH_3COCH_3) to track the fuel concentration alone. Recently Stöhr et al. [26] added acetone to track the fuel mole fraction within a swirl flame in the DLR Gas Turbine Model Combustor (GTMC) while they simultaneously tracked the flame boundary by recording the OH planar laser-induced fluorescence (PLIF) signal. However they had no way to track the oxygen (O_2) so they could not measure the flame index or the local fuel–air ratio. They did show that the acetone marker was a good indicator that fuel mole fraction just ahead of the flame surface varied by large amounts. They could not determine whether or not the mixture lies within the flammability limits. Their scatter plots indicated that instantaneous temperatures were not bimodal as would be expected in premixed combustion. Nor were their scatter plots expected for a pure non-premixed flame. They concluded that "results demonstrate a fast mixing of fuel and air but flames cannot be regarded as uniformly premixed but should be classified as partially premixed." In a related study Meier et al. [27] showed that flamelets exist because they observed thin layers in their CH PLIF images, but they could not determine which layers were premixed.

2. Objectives

There have been no previous measurements of flame index, ξ, because appropriate diagnostics were not developed prior to the present project. Raman scattering has not proved to be a viable way to measure the directions of the gradients of the fuel and O_2 mass fractions that appear in Eq. (1). Two-dimensional images are required and there have been no reported simultaneous 2-D Raman images of fuel and O_2 that have sufficient spatial resolution to resolve flamelets within intense turbulence. The only viable approach is to record the planar laser-induced fluorescence (PLIF) from appropriate tracer gases.

Therefore the first objective was to select two tracer gases and run CHEMKIN in order to compute the signs of the maximum gradients of the fuel mass fraction, the O_2 mass fraction, and the tracer gas signals. Section 3 describes the three types of flames that were selected for the computations: laminar premixed, laminar