Combustion and Flame 159 (2012) 3353–3357

Contents lists available at SciVerse ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Brief Communications

A priori investigation of PDF-modeling assumptions for a turbulent swirling bluff body flame ('SM1')

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ARTICLE INFO

Article history:
Received 13 October 2011
Received in revised form 23 February 2012
Accepted 9 June 2012
Available online 8 August 2012

Keywords:
Progress variable
PDF modeling
Statistical independence
Swirling flame

1. Introduction

The present study deals with a direct statistical analysis of experimental scatter data for the swirling non-premixed methane/air bluff-body flame 'SM1' [1–6], in the context of the popular non-premixed combustion modeling concept of mixture fraction and progress variable. For the flame studied, the scatter data in composition space, taken at fixed locations in physical space, is similar to what is observed in jet type flames with a substantial amount of local extinction, such as Sandia Flames E and F [7–9] in that there is strong deviation from steady-flamelet type lines in composition space (corresponding to little or no local extinction). A study on the experimental data of Sandia Flames D–F as discussed in [10] led to the formulation of the double conditioned CMC approach, using sensible enthalpy as progress variable. The latter is a measure for the deviation from the mentioned flamelet type lines or, equivalently, for the amount of local extinction. However, flame SM1 is different from jet type flames in that transported PDF simulations indicate that, close to the burner inlet, the deviations from flamelet type lines in composition space are not due to slower chemistry, caused by turbulence–chemistry interaction, but rather due to 'large scale' mixing of hot combustion products with air or fuel in the recirculation region behind the bluff body [11]. This motivates the present work. The a priori study on experimental data for SM1 reveals that using a mixture fraction–progress variable modeling approach in a RANS framework can lead to potentially large errors in the mean reaction rate. Different definitions of the progress variable and different shapes of the presumed joint PDF (product of marginal PDFs, using the assumption of statistical independence), are addressed.

2. Progress variable definitions and presumed-PDF modeling assumptions

In turbulent non-premixed combustion modeling, the PDF (probability density function) of mixture fraction Z models the effect of turbulence on chemistry. In a reduced scalar approach (e.g., FGM [12], FPI [13], REDIM [14] and ADF-PCM$_\chi$ [15], flamelet–progress variable (FPV) [16]), the 'progress' of the reaction is modeled by e.g., a 'progress variable' (c [15–17] or sensible enthalpy [10]) or a 'reaction progress parameter' λ [18] [in [15], a third additional property, the scalar dissipation rate χ, is also considered]. In the literature, many definitions appear for the progress variable, including: reduced temperature [18], sensible enthalpy [10] or a linear combination of species mass fractions [16,17,19–21]. In the present study, we refer to the latter with the symbol Y_c and choose $Y_c = Y_{CO_2}$. The definition $Y_c = Y_{CO_2} + Y_{CO}$ [19,22] leads to a better monotonicity of temperature and species in regions where CO_2 decomposes into CO, but this does not affect the observations in the study at hand (not shown).

Unless a transported PDF approach [23] is adopted, assumptions are commonly invoked on the shape of the PDF and on statistical (in)dependence of Z and c or Z and λ. For instance, presumed

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0010-2180/$ - see front matter
http://dx.doi.org/10.1016/j.combustflame.2012.06.018

PDF assumptions are introduced in the RANS modeling frameworks used in [19,24]. The use of a progress variable in the context of presumed PDF modeling is mainly based on two assumptions: (i) statistical independence between Y_c and Z, and (ii) modeling of the marginal PDFs of Z and Y_c based on their mean and variance.

Marginal PDF shapes. The probability density function (PDF) of Z at point $\boldsymbol{x}$ and time t, $P(Z; \boldsymbol{x}, t)$, is often approximated by a β-distribution based on the mean mixture fraction $\widetilde{Z}(\boldsymbol{x}, t)$ and mixture fraction variance $\widetilde{Z''^2}(\boldsymbol{x}, t)$ [25]. For $P(c; \boldsymbol{x}, t)$, and $P(\lambda; \boldsymbol{x}, t)$ different shapes have been used. Although recently the 'statistically most likely distribution' has been introduced [20,21], δ- and β-functions are still the most commonly used. In order to use a β-function in (ii), the progress variable must have the same range of values everywhere. Therefore, it is advantageous to normalize the progress variable such that the range becomes [0–1] [26]. Normalization of Y_c can also help in satisfying assumption (i) [19,24]. In [19,24,26], $Y_c(Z)$ is normalized with the equilibrium value $Y_{c,eq}(Z)$. Here, we normalize the progress variable $Y_c(Z)$ with $Y^{(\mathrm{fs})}_{CO_2}(Z)$, the value on the flame sheet (Burke–Schumann model) going through $Y^{(\mathrm{fs})}_{CO_2}(Z_{\mathrm{st}}) = 0.1513$ at $Z_{\mathrm{st}} = 0.054$:

$$c(Z, Y_c) \equiv Y_c / Y^{(\mathrm{fs})}_c(Z) = Y_{CO_2} / Y^{(\mathrm{fs})}_{CO_2}(Z). \tag{1}$$

Whether the normalization is based on equilibrium values $Y_{c,eq}(Z)$ or flame sheet values $Y^{(\mathrm{fs})}_{CO_2}(Z)$ is not essential for the study at hand. It merely affects the absolute values of $c(Z)$ (especially at the rich side), not the global observations.

Joint PDF and statistical (in)dependence. Considering the joint PDF, statistical independence of the variables is usually assumed: $P(Z, c) = P(Z) \cdot P(c)$ or $P(Z, \lambda) = P(Z) \cdot P(\lambda)$, assumption (i). The general joint PDF definition involves a conditional PDF, though:

$$P(Z, c; \boldsymbol{x}, t) = P(Z; \boldsymbol{x}, t) \cdot P(c|Z; \boldsymbol{x}, t). \tag{2}$$

Comparison of conditional PDFs for different values of Z thus indicates to what extent assumption (i) of statistical independence prevails. Figure 2 reveals that the normalization (1) leads to plateaus of constant c-values for non-premixed flamelets[1] at the lean side and at the rich side (since the corresponding Y_{CO_2} profiles have shapes similar to the flame sheet). Only around stoichiometry there is a non-linear relationship between c and Z. A limited number of measurements reveal Y_{CO_2} values, higher than $Y^{(\mathrm{fs})}_{CO_2}(Z)$. In the normalization procedure, the value of c for these points has been clipped to 1. They could also have been ignored in our analysis, if interpreted as 'outliers'. The clipping does not affect the global analysis at hand, given the fact that the number of points clipped is negligible in the amount of experimental data.

In [18], the 'reaction progress parameter' λ quantifies the reaction 'progress':

$$\lambda(Z, Y_c) \equiv \left\{ Y^{(\mathrm{stoich})}_c \right\}_{\text{flamelet 'F'}} \quad \text{such that} \quad (Z, Y_c) \text{ is on flamelet 'F'}. \tag{3}$$

In this definition, all points in (Z, Y_c) or (Z, c) space are assumed to lie on (stable or unstable) steady non-premixed flamelets and λ denotes the value of the (traditional) progress variable Y_c at stoichiometry on that steady non-premixed flamelet. As long as the real flame structure corresponds to a collection of steady non-premixed flamelets, λ is constant along each flamelet and as such becomes statistically independent of Z. In [28], still another progress variable is defined, based on the enthalpy of formation integrated over Z-space, making it statistically independent of Z.

Both definitions of the progress variable c and of the reaction progress parameter λ are useful with respect to condition (i) for presumed PDF modeling of flame SM1 if the composition in (Z, Y_{CO_2}) space mainly corresponds to steady turbulent non-premixed flamelets. It is shown in Section 4 that introducing such progress variables in a priori studies of the experimental data helps to identify steady non-pemixed flamelet structures.

Progress variable transport equation. With respect to c and λ, the definitions of normalized progress variables or reaction progress parameters are useful in order to satisfy (i) and (ii) in the context of presumed PDF modeling. However, at some point the modeling of the mean or filtered value, and possibly the variance, of c or λ is required. The transport equations for these quantities contain non-negligible terms that are harder to model than the corresponding terms in the standard transport equations for Y_c [21,29]. In [21], in the context of LES, solving the transport equation for λ is avoided by assuming a 'statistically most likely distribution' for $P(\lambda)$. In [19,24], in the context of RANS simulations, an assumption is formulated for the mean progress variable (i.e., the first moment of the PDF): $\overline{c|Z} = \bar{c}$. This assumption is less stringent than complete statistical independence, $P(c|Z) = P(c)$, while solving the transport equation for the mean progress variable $\bar{c}$ is avoided. Instead, the transport equation for the mean non-normalized progress variable $\widetilde{Y_c}$ is solved and $\bar{c}$ is reconstructed afterwards from $\widetilde{Y_c}$. It is illustrated below, though, that for the flame at hand the assumption $\overline{c|Z} = \bar{c}$ is questionable.

A priori study. The study at hand concerns a direct analysis of experimental data in the sense of RANS modeling. As mentioned, the scatter in the experimental data of flame SM1 is primarily caused by 'large scale' mixing of hot combustion products with air or fuel in the recirculation region behind the bluff body [11], not by local extinction (or lack in 'progress' of the reaction). It is illustrated below that commonly made assumptions in RANS frameworks do not prevail: Z and c or Z and λ are not statistically independent; and $\overline{c|Z} \neq \bar{c}$.

3. Marginal PDFs

Figure 1 shows the marginal PDFs of Z, c and λ as retrieved from the experimental data at $x/D = 0.4$ (which is close to the bluff body, inside the recirculation region). The results at other axial locations are similar (not shown). The radial locations have been chosen close to the shear zone because there the mixing is the strongest and the largest differences are expected (r is the distance from the symmetry axis and $R = D/2$). In order to have a sufficient amount of samples in each bin, the experimental data has been divided for each scalar (Z, c or λ) into 25 equally sized bins. The analysis presented below has been confirmed to remain valid when the bins have only half the size. The experimental PDFs of c and λ include non-zero values at $c = 1$ and $\lambda = 1$ due to the clipping of experimental measurements above the flame sheet in (Z, Y_c) space, but this is not relevant in the discussion at hand. [Note that λ has been normalized with $\lambda_{max} = Y^{max}_{CO_2}(Z_{stoich}) = 0.1513$ in order to make the range of all horizontal axes equal to [0–1].].

The corresponding β-PDFs, with the same values for mean and variance as retrieved from the experimental data, are shown to be good approximations for the marginal PDF of Z, while for c and λ the strong deviations observed at some locations indicate that the β-PDF assumption is not generally applicable for these variables. The vertical lines at the mean value represent the δ-PDF. In general, the δ-PDF assumption is clearly insufficient to model any of the marginal Z, c and λ PDFs. These observations are in line with [20]: higher order statistical information is needed to represent complex PDFs (highly skewed or bimodal PDFs).

We recall that the experimental data is treated here in a RANS modeling sense. The above observations do not give information about the validity of models for the shape of the marginal filtered

[1] The steady non-premixed flamelets represented in Fig. 2 were calculated in the axisymmetric opposed-flow configuration, with Warnatz mechanism [27], assuming unity Lewis number, for different strain rates (a = 100,320,392 s^{-1}).