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Effects of dissipation rate and diffusion rate of the progress variable on local fuel burning rate in premixed turbulent flames

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ABSTRACT

The validity of the premixed flamelet equations and the dependence of the fuel burning rate on the parameters involved in these equations have been investigated using a large series of direct numerical simulations of turbulent premixed flames in the thin reaction zones (TRZ) and the distributed reaction zones (DRZ) regimes. Methane, toluene, *n*-heptane, and *iso*-octane fuels were considered over a wide range of unburnt conditions and turbulence characteristics. Flames with unity and non-unity Lewis numbers were investigated separately to isolate turbulence-chemistry interaction from differential diffusion effects. In both cases, the flamelet equations, which rely on the assumption of a thin reaction zone, are locally valid throughout the TRZ regime, more precisely up to a Karlovitz number at the reaction zone of 10 (based on the definition used in this paper). Consistent with this result, in the unity Lewis number limit, the fuel burning rate is strongly correlated with the dissipation rate of the progress variable, the only parameter in the flamelet equations. In the non-unity Lewis number case, the burning rate is a strong function of both the dissipation rate and the diffusion rate, both of which are parameters in the flamelet equations. In particular, the correlation with these parameters is significantly better than with curvature or tangential strain rate.

1. Introduction

Turbulent premixed flames play a major role in modern internal combustion engines and gas-turbine combustors. These premixed flames often involve large hydrocarbon fuels and typically fall in the thin reaction zones (TRZ) regime [1–5]. To promote an efficient engine design process, a better understanding of turbulent premixed flames in this regime, and with such fuels, is desirable.

In previous studies [6,7], we investigated, with direct numerical simulations (DNS), $n\text{-}C_7H_{16}$/air premixed turbulent flames at high Karlovitz number (TRZ regime), with and without differential diffusion. The following results were identified:

(1) largely thickened preheat zone
(2) thin reaction zone
(3) large fluctuations around $\langle \dot{\omega}_F | c \rangle$
(4) for unity Lewis numbers:

$$\langle \dot{\omega}_F | c \rangle \approx \dot{\omega}_{F,\mathrm{lam}}(c), \tag{1}$$

(5) for non-unity Lewis numbers:

$$\langle \dot{\omega}_F | c \rangle \not\approx \dot{\omega}_{F,\mathrm{lam}}(c), \tag{2}$$

where $\dot{\omega}_F$ is the fuel burning rate, and c is a progress variable. $\langle \cdot | \psi \rangle$ denotes the mean conditional to the variable ψ. Lapointe et al. recently obtained similar results for *n*-heptane/air (over a wider range of Karlovitz numbers) [8,9], *iso*-octane/air [9], and toluene/air [9] flames with both high and low unburnt temperatures. Consistent results were also obtained for *iso*-octane/air flames in the TRZ regime over a wide range of pressures [10]. (While similar results are expected for all heavy hydrocarbon fuels, extension to certain light fuels such as hydrogen may not be warranted.)

It is important to note that broadened preheat zone (point 1), and yet thin reaction zone (point 2), have been observed beyond the traditional boundaries of the TRZ regime (*i.e.* at Karlovitz numbers higher than theoretically predicted [11]) [12]. Burning rate

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fluctuations (point 3) have also been identified in various other DNS studies [13–16]. Such source term fluctuations in turbulent flames have commonly been attributed to stretching effects, *i.e.* effects of curvature and strain rate [13,16–19]. However, these results were obtained at relatively low Karlovitz numbers, namely in the wrinkled/corrugated flamelet regimes and at the lower limit of the TRZ regime. In contrast, no strong correlation was identified between burning rate and strain rate or curvature at larger Karlovitz numbers [7].

The effect of the dissipation rate

$$\chi = 2\alpha|\nabla c|^2, \tag{3}$$

with α the thermal diffusivity, on the burning rate in premixed turbulent flames has also been previously discussed in the literature. For instance, Bray [20], under BML assumptions, showed that the mean (Reynolds-averaged) source term should be proportional to the mean dissipation rate. Lipatnikov et al. [21] recently showed, using DNS data, that this result is valid in the wrinkled/corrugated flamelet regimes. Bray's model has later been improved for application to both Reynolds-averaged Navier–Stokes simulations (RANS) and large eddy simulations (LES) (*e.g.*, Refs. [22–26]). In conditional mean closure (CMC) methods, the scalar dissipation rate is an essential term that needs closure [27,28]. Veynante and Vervisch [29] also discuss the importance of the scalar dissipation rate for turbulent combustion modeling. Nevertheless, none of these models uses the dissipation rate to capture the burning rate fluctuations (only the mean or filtered burning rate).

In the absence of differential diffusion, Kolla [30] showed that, if the species mass fractions are only a function of the progress variable, then

$$\dot{\omega}_c \frac{\partial Y_i}{\partial c} = \frac{\rho\chi}{2}\frac{\partial^2 Y_i}{\partial c^2} + \dot{\omega}_i, \tag{4}$$

where Y_i is the ith species mass fraction, ρ is the density, and $\dot{\omega}_i$ is the chemical source term of species i. In analogy with non-premixed flamelet equations, this constitutes a *premixed flamelet equation*. Nguyen et al. [31] also derived a similar equation and showed the importance of the progress variable dissipation rate. Recently, Lapointe and Blanquart [9] investigated a wide range of turbulent premixed flames in the TRZ and the distributed reaction zones (DRZ) regimes. They showed that the burning rate fluctuations are strongly correlated with the dissipation rate on the iso-temperature corresponding to the peak burning rate. It is important to highlight that these results were obtained in the absence of differential diffusion.

The inclusion of differential diffusion effects in *non-premixed* flamelet equations has been the subject of multiple studies [32–35] starting with Pitsch and Peters [36]. By considering a progress variable instead of a mixture fraction and using a coordinate transformation similar to Xuan et al. [34], we derived 3D *premixed* flamelet equations with non unity Lewis numbers in Ref. [37]. In analogy to the non-unity Lewis number non-premixed case, an additional parameter was identified in the premixed flamelet equations, namely the diffusion rate of the progress variable, $\nabla \cdot (\rho\alpha\nabla c)$. To the best of the authors' knowledge, the dependence of burning rate fluctuations on this quantity in turbulent premixed flames has never been investigated.

In light of the above discussion, the first objective is to test the validity of the premixed flamelet equations in turbulent premixed flames across the TRZ regime up to the DRZ regime over a wide range of unburnt conditions and mixtures (with particular attention to large hydrocarbon fuels). Both unity and non-unity Lewis number cases will be considered. A value for the largest Karlovitz number at the reaction zone for which the equations are valid can then be provided as a by-product. Note that the validity of flamelet equations in turbulent flames was recently tested by Scholtissek et al. [35] but only for non-premixed flames. The second objective is to assess if burning rate fluctuations can be locally attributed to variations in the parameters from the flamelet equations. It is beyond the scope of this work to provide a closed model to be implemented in future LES. The focus is placed entirely on providing physical and mathematical explanations to these burning rate fluctuations.

The paper is organized as follows. The non-unity Lewis number premixed flamelet equations are reviewed in Section 2. An overview of the DNS data set on which the analysis is performed is presented in Section 3. For the analysis, the unity Lewis number limit is considered first in Section 4. The analysis is then repeated in Section 5 for the non-unity Lewis number cases and differential diffusion effects are highlighted. Finally, a summary and conclusions are provided in Section 6.

2. One-dimensional flamelet equations

The one-dimensional flamelet equations presented in this section, which were first introduced in Ref. [37], are the premixed equivalent of the non-premixed flamelet equations derived in Xuan et al. [34]. For complete details of the derivation, the reader is referred to [37, Chapter 7].

The premixed flamelet equations result from the following coordinate transformation applied to the species transport and temperature equations:

$$(x_1, x_2, x_3, t) \rightarrow (c(x_1, x_2, x_3, t), c_2(x_1, x_2, x_3, t), c_3(x_1, x_2, x_3, t), \tau), \tag{5}$$

with

$$\nabla c \cdot \nabla c_2 = 0, \qquad \text{and} \qquad \nabla c \cdot \nabla c_3 = 0, \tag{6}$$

i.e. the variables c_2 and c_3 lie in the surface of constant c. Note that these variables can be curvilinear. The progress variable c is considered to be a linear combination of species mass fractions Y_j in the derivation, *i.e.* $c = \sum_{j=1}^{N} b_j Y_j$, where the b_j's are arbitrary coefficients and N is the number of species. For the results shown in Sections 4 and 5, $c = Y_{H_2} + Y_{H_2O} + Y_{CO} + Y_{CO_2}$. (Note that we did not normalize the progress variable to unity. Hence, it ranges from 0 to 0.25 for the present n-C_7H_{16}/air flames.)

The next step consists of assuming that, in the vicinity of the reaction zone, all tangential derivatives ($\partial/\partial c_k$) are negligible compared to the normal derivatives ($\partial/\partial c$). It is further assumed that the dependence on τ in the transformed coordinate system is negligible. Note that the coordinate c is still a function of time t. These assumptions are expected to be more valid at lower Karlovitz number (thin reaction zones) than at high Karlovitz number (distributed reaction zones). This will be assessed in Sections 4 and 5. These two assumptions will be used (and tested) in the rest of this paper and are therefore listed here for clarity:

$$\partial/\partial c_k \ll \partial/\partial c, \quad \text{for} \quad k = 2, 3, \tag{7}$$

$$\partial/\partial\tau = 0. \tag{8}$$

With these assumptions (note that no assumption is made on the species Lewis numbers), the flamelet equations for the mass