Combustion and Flame 161 (2014) 1547–1557

Contents lists available at ScienceDirect

Combustion and Flame

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

An *a priori* model for the effective species Lewis numbers in premixed turbulent flames

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ARTICLE INFO

Article history:
Received 26 July 2013
Received in revised form 12 December 2013
Accepted 13 December 2013
Available online 17 January 2014

Keywords:
Non-unity Lewis number
Turbulent premixed flame
Scalar transport
Turbulent mixing
Hydrogen

ABSTRACT

An *a priori* model for the effective species Lewis numbers in premixed turbulent flames is presented. This *a priori* analysis is performed using data from a series of direct numerical simulations (DNS) of lean ($\phi = 0.4$) premixed turbulent hydrogen flames, with Karlovitz number ranging from 10 to 1562 (Aspden et al., 2011). The conditional mean profiles of various species mass fraction versus temperature are evaluated from the DNS and compared to unstretched laminar premixed flame profiles. The turbulent flame structure is found to be different from the laminar flame structure. However, the turbulent flame can still be mapped onto a laminar flame with an appropriate change in the Lewis numbers of the different species. A transition from "laminar" Lewis numbers to unity Lewis numbers as the Karlovitz number increases is clearly captured. A model for those effective Lewis numbers with respect to the turbulent Reynolds number is developed. This model is derived from a Reynolds-averaged Navier–Stokes (RANS) formulation of the reactive scalar and temperature balance equations. The dependency of the effective Lewis numbers on the Karlovitz number instead of the Reynolds number is discussed in this paper. Unfortunately, given that the ratio of the integral length to the laminar flame thickness is fixed throughout this series of DNS, a change in the Karlovitz number is equivalent to a change in the Reynolds number. Incorporating these effective Lewis numbers in simulations of turbulent flames would have several impacts. First, the associated laminar flame speed and laminar flame thickness vary by a factor of two through the range of obtained effective Lewis numbers. Second, the turbulent premixed combustion regime diagram changes because a unique pair of laminar flame speed and laminar flame thickness cannot be used, and a dependency on the effective Lewis numbers has to be introduced. Finally, a turbulent flame speed model that takes into account these effective Lewis numbers is proposed.

1. Introduction

Lean hydrogen low-swirl burners have recently become an interesting solution for clean energy production [1]. However, the flame produced in the combustion chamber has a different shape than that obtained with natural gas or propane. Stability issues are observed and the noise level is too high [2]. The combustion chamber has to be redesigned to tackle those issues. This process will require large eddy simulations (LES) capable of reproducing accurately the behavior of the flame. However, as of today, the models used are either too computationally expensive for the industry or simply incapable of capturing the turbulent lean hydrogen flame's behavior. These issues come from the fact that hydrogen has a low Lewis number ($Le = 0.3$) in a lean hydrogen/air mixture. While a large body of work has been done on simulating and modeling turbulent premixed flames [3–10], most of these studies consider methane as the fuel (which has a close to unity Lewis number). Unfortunately, fuels found in industrial applications, as described for the low-swirl burner, rarely have unity Lewis numbers. As an additional example, the Lewis number of *n*-dodecane, a surrogate for kerosene, is approximately 3.5 in air. There is a need to extend models to simulate accurately turbulent premixed flames with non-unity Lewis numbers, especially at high Karlovitz numbers.

LES of turbulent flames requires chemistry reduction and probability density function (PDF) modeling efforts. The focus in this paper is put on the chemistry reduction. Note that chemistry reduction is independent from the LES closure and is also relevant to Reynolds-averaged Navier–Stokes simulations (RANS) and direct numerical simulations (DNS). Chemistry reduction can be done by the use of reduced chemical mechanisms, bringing the number of transported species down to a tractable number [11], or by tabulation, reducing the number of transported scalar variables to one or two [7,12]. The latter method is computationally very attractive for obvious reasons. However, the validity of tabulated chemistry lies

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http://dx.doi.org/10.1016/j.combustflame.2013.12.014

on an important hypothesis: the turbulent flame structure is assumed to be similar to that of an unstretched laminar flamelet. To investigate this hypothesis, Aspden et al. [13] recently performed a series of DNS of lean ($\phi = 0.4$) premixed hydrogen flames at Karlovitz numbers ranging from 10 to 1526. Their results clearly show that the turbulent flame structure varies significantly between the lowest and the largest *Ka* flames. At first sight, these results seem to invalidate the hypothesis on which tabulated chemistry relies.

Another challenge for tabulated chemistry is the choice of Lewis numbers. For non-premixed turbulent flames, tabulation is usually done with unity Lewis number flamelets, even when the species have Lewis numbers far from unity [14–16]. The underlying reason is that at high turbulence levels, diffusion of species and temperature is dominated by turbulent mixing, resulting in an effective unity Lewis number. This gives good results at sufficiently high turbulence, as experimentally observed [17,18]. To the best of the authors' knowledge, there is no premixed flame experiment equivalent to those conducted in Refs. [17,18] in the literature. With their series of premixed turbulent flames, Aspden et al. [13] observed that the largest *Ka* flame has a structure comparable to that of a methane flame, *i.e.* the flame behaved as an effective unity Lewis number flame. This is consistent with the previous argument for non-premixed flames. However, for premixed turbulent flames, chemistry tabulation is generally done by computing flamelets with full transport [19] or constant "laminar" Lewis numbers [7]. There is clearly an inconsistency between what is done for premixed and non-premixed chemistry tabulation.

Following these observations, the objectives of this work are as follows: (1) to determine if turbulent premixed flames can be mapped onto unstretched laminar flamelets, (2) to identify what Lewis numbers should be used to tabulate unstretched laminar flamelets, (3) to derive an *a priori* model for the effective Lewis numbers in premixed turbulent flames, and (4) to investigate the consequences of these effective Lewis numbers. Note that only premixed flames are considered in this work. Furthermore, as mentionned earlier, the focus is placed on the chemistry tabulation and not on sub-grid scale closure for use in RANS or LES.

Section 2 presents the flame structure obtained from the DNS data of Aspden et al. and compares it to corresponding laminar unstretched flamelets. Section 3 derives an *a priori* model from simplified species and temperature balance equations. Section 4 compares the model against the effective Lewis numbers computed from the DNS. Section 5 discusses different approaches to derive a model for these effective Lewis numbers. A Reynolds number versus a Karlovitz number dependency is especially emphasized. Finally, Section 6, in addition to discussing the model's sensitivity, applicability, and practical use, presents the impacts of the effective Lewis numbers on the laminar flame speed and the laminar flame thickness, the effective Karlovitz number and the regime diagram, and the turbulent flame speed models.

2. Turbulent flame structure

In this work, the flame structure from the series of direct numerical simulations performed by Aspden et al. [13] is compared to the structure of laminar unstretched flamelets. A schematic diagram of the flow configuration used for the DNS is presented in Fig. 1. The complete set of parameters describing the DNS cases can be found in Ref. [13] and are summarized in Table 1. The reactants are a lean ($\phi = 0.4$) hydrogen-air mixture. A reduced version of GRI-2.11 was used as the chemical mechanism (9 species, 27 reactions; all carbon-based species and associated reactions were removed). Soret and Dufour effects as well as radiation were not included in the DNS [13]. As confirmed in Ref. [13] and shown in Fig. 2, the transition from the thin reaction zone to the broken reaction/distributed burning zone is covered by the simulation cases.

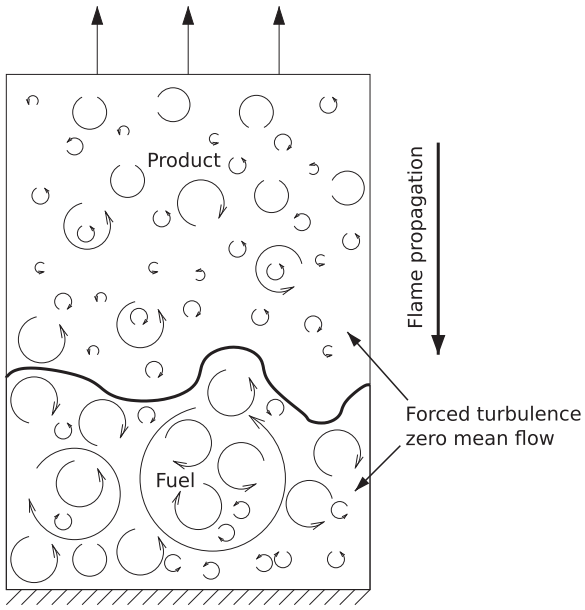

Fig. 1. Schematic diagram of the flow configuration used by Aspden et al. [13]. Diagram taken from Ref. [13].

The laminar flame counterparts are simulated using FlameMaster [22]. The equivalence ratio is fixed to 0.4; the same chemical model as in the DNS is used; and Soret and Dufour effects and radiation heat losses are ignored.

The conditional means of the mass fractions with respect to temperature $\langle Y_i|T\rangle$ are calculated for several instantaneous snapshots of the established (statistically steady) propagating flame. Figure 3 shows the conditional mean hydrogen mass fraction as a function of temperature for cases A through D. The temperature is used here as a progress variable. Are also shown in Fig. 3, the profiles for laminar unstretched flamelets with full transport [20,21] and unity Lewis numbers. The "full transport" and "unity Lewis numbers" laminar flames correspond to limiting cases of purely laminar and fully turbulent premixed flames, respectively. A clear trend is observed: the DNS profiles gradually move from the purely laminar towards the fully turbulent limiting cases. It is important to stress that all DNS data are "bracketed" by these two limiting cases. As mentioned earlier, one of the objectives of this work is to model this transition between the purely laminar to the fully turbulent flame structure.

The effects of thermo-diffusive instabilities are revealed by the presence of hot-spots in Fig. 3, *i.e.* by the extension of the DNS profiles to temperatures higher than the adiabatic flame temperature ($T_{ad} \approx 1400$ K). However, the present analysis is aimed to address the turbulent transport problem only. Unfortunately, this transport is influenced by these thermo-diffusive instabilities. While these instabilities have an important impact on laminar flames [2], they are expected to be less important as turbulence increases, *i.e.* as preferential diffusion becomes negligible due to turbulent mixing. This is observed for the highest *Ka* DNS case (D). The qualitative behavior of the turbulent flame structures shown in Fig. 3 and, as it will be presented in Section 4, the good agreement of the proposed model suggest that these instabilities have limited impact on the statistical mean structure. As the hot spots and the super-adiabatic temperatures are not a consequence of turbulent transport (of concern in this work) and are entirely due to those instabilities, they are not considered in this work. Computing the conditional mean as $\langle Y_i|T\rangle$ instead of $\langle T|Y_i\rangle$ allows one to isolate these hot spots.