



Assessment of differential diffusion effects in flamelet modeling of oxy-fuel flames

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ABSTRACT

The modeling of differential diffusion in flamelet-based approaches is analyzed in a turbulent non-premixed oxy-fuel flame experimentally investigated by Sevault et al. (2012). The flamelet models considered are the unity Lewis number flamelet (ULNF) model proposed by Peters (1986), the variable Lewis number flamelet (VLNF) model presented by Pitsch and Peters (1998) and a recently proposed model where the influence of turbulence on variable Lewis numbers is incorporated (NLVNF, Wang, 2016). The suitability of the different manifold-based approaches is studied by means of a *prior* analysis based on the experimentally data derived from Raman/Rayleigh measurement and a fully coupled Large-Eddy Simulation (LES). In both cases, the Bilger mixture fraction and the progress variable are chosen as the flamelet parameters in order to be consistent with the experiments. The *prior* analysis confirms the presence of strong differential diffusion effects in the reaction zone and near the fuel nozzle, which decrease towards the fuel-rich flame zone and further downstream. In general, the NLVNF model yields an improvement in the representation of the flame structure compared to the ULNF and VLNF models and this model is able to capture the transition to the unity Lewis number behavior. However, discrepancies in predicting all species and the temperature profiles still remain. These results are further quantified through the use of the Wasserstein metric, which has recently been introduced as a diagnostic tool for combustion model validation. In the LES, all major species are transported for the calculation of the Bilger mixture fraction. The tabulated major species mass fractions reveal contradicting findings compared to the *prior* analysis. The transported species are in better agreement with the experimental data than the tabulated ones, which is attributed to the direct consideration of turbulent and molecular transport.

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1. Introduction

“Differential diffusion” is a term that characterizes the separate evolution of initially perfectly correlated scalars in a turbulent or laminar flow caused by differences in the molecular diffusive properties between species. The first observation of differential diffusion in a methane diffusion flame was reported by Bilger [1]. Experimental and numerical investigations using reactive and also non-reactive flows followed; an overview can be found in [2]. It is well known that differential diffusion is significant in flames with substantial amounts of H₂ ($Le < 1$) or higher hydrocarbons ($Le \gg 1$).

This is particularly true in laminar flames. In turbulent flames, differential diffusion is dampened by turbulent motion. Therefore, in many turbulent flames, unity Lewis number behavior for all species has been observed and confirmed, particularly for CH₄/air flames [3], DME/air flames [4,5] and recently also for a CH₄/oxy-fuel flame [6,7]. However, differential diffusion has been observed in other turbulent diffusion flame studies. In an experimental study of turbulent H₂/air diffusion flames [8], differential diffusion was identified in the near-nozzle region and at low Reynolds numbers. A recent experimental study of turbulent CH₄/oxy-fuel flames also confirmed the presence of differential diffusion [9]. Pitsch [10] indicated the following three phenomena relevant for turbulent flames: (i) laminar structures within the mixing layer in the near-nozzle field, (ii) large molecular diffusivities of single species and (iii) scale separation when the mixing layer width is small compared to the Kolmogorov scale. In addition, the position

Acronyms: ULNF, unity Lewis number flamelet; VLNF, variable Lewis number flamelet; NLVNF, non-linear variable Lewis number flamelet.

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of the turbulent/non-turbulent interface relative to the reaction zone was recently identified as relevant for the existence of differential diffusion in shear flows [7]. Although these processes have clearly been associated with the occurrence of differential diffusion in turbulent flames, only few models are able to capture some or all of these effects, involving the competition between molecular diffusion and turbulence. The conditional moment closure (CMC) model was extended such that it explicitly contains a term in the species and enthalpy transport equation responsible for differential diffusion [11]. However, a similar approach is not yet available for tabulated chemistry as used in flamelet models.

Hence, the present paper aims to advance knowledge about differential diffusion by assessing a hierarchy of flamelet models to capture significant differential diffusion effects in a CH₄/oxy-fuel flame that was experimentally investigated by Sevault et al. [9]. In that investigation, differential diffusion was shown to dominate around stoichiometric conditions in all species profiles. Approximate unity Lewis number behavior was found for many species such as H₂, CO₂ and CO in the fuel-rich part of the flame. This was confirmed by comparing experimental data and simulation results for opposed-flow diffusion flames using representative strain rates either accounting or not for differential diffusion. Garmory and Mastorakos [12] confirmed the presence of differential diffusion in LES of this flame when applying a newly proposed unstructured CMC method. Since a unity Lewis number diffusion model was used, not all species could be predicted equally well. In a first attempt to model differential diffusion in this flame, Han et al. [13,14] applied a modified flamelet model [15] in a Reynolds-averaged Navier–Stokes (RANS) framework. The model uses the mixture fraction and scalar dissipation rate as parameters and accounts for differential diffusion as well as its interaction with turbulent mixing. A significant improvement was achieved compared to unity Lewis number modeling, particularly for the profile of the CO and CO₂ mass fraction. Despite the improvements in CO, significant differences still persisted in this species and correspondingly in the profiles of the differential diffusion parameter.

In the present study, the flamelet/progress variable (FPV) model [16,17] is applied, in which different reaction-diffusion manifolds are used that are parametrized by the mixture fraction Z and the progress variable Y_c . This allows for a detailed *prior* analysis since both quantities can be evaluated directly from the experimental Raman/Rayleigh data. For a fully coupled LES of jet flames, the FPV approach has been shown to be a feasible choice [4,6,7].

For the investigation of modeling differential diffusion in this flame, three main aspects are considered. First, the experimental data including the associated measurement uncertainties are analyzed with respect to the sensitivity of the flamelet and differential diffusion parameters. Second, the experimental data are compared to the manifolds by means of a *prior* analysis. Finally, a fully coupled LES is performed in terms of an *a posteriori* analysis and these results are compared to measurements.

All manifolds are generated using 1D flamelet solutions, which only differ in the treatment of the diffusion term:

- (i) unity Lewis number assumed [18];
- (ii) differential diffusion accounted for by variable Lewis numbers [19];
- (iii) influence of local turbulence considered by using effective Lewis numbers [15].

The remainder of this paper is structured as follows. The numerical approach is outlined in Section 2 and measurement uncertainties are discussed in Section 3. Results of the *prior* analysis as well as of the *a posteriori* LES are presented and discussed in Section 4. Section 5 summarizes the work.

2. Investigated setup and numerical approach

In the following analysis we consider one flame of the flame series experimentally investigated by Sevault et al. [9]. The series used non-piloted, non-premixed turbulent oxy-fuel flames. The Damköhler number of all flames, evaluated with the mean jet time scale and the chemical time scale calculated following Peters [20], was found to be greater than 1. The chosen flame is configuration B1 which was found to be fully burning and attached to the nozzle. The burner consists of two concentric tubes placed in a wind tunnel with a cross-section of 250 mm × 250 mm. The oxidizer flows through the outer tube with an inner diameter of 96.5 mm, and the fuel enters through the inner tube with a diameter of 5 mm and 0.5 mm wall thickness. The oxidizer is composed of 32 vol-% O₂ and 68 vol-% CO₂, whereas the fuel consists of 45 vol-% CH₄ and 55 vol-% H₂, which yields a stoichiometric mixture fraction of $Z_{st} = 0.0535$, evaluated from the composition in the oxidizer and fuel streams. All streams are conditioned to 294 K. The oxidizer inlet velocity is 0.622 m/s and the fuel has a fully developed turbulent inlet profile with a jet velocity of 78.6 m/s, corresponding to a Reynolds number of 12,000.

In the following, only non-premixed manifolds are considered. The analysis shown in Supplementary Material A confirms that premixed manifolds are not suitable for the flame considered. This can mainly be attributed to the narrow flammability range and consequently to the inadequate representation of the coupling between mixing and reaction in fuel-rich regions. The diffusion flamelet models applied here are described in Section 2.1. To allow for a systematic comparison, a *prior* analysis is performed first, which is described in Section 2.2, the fully coupled LES approach is discussed in Section 2.3.

2.1. Flamelet approach

As mentioned above, the FPV framework [16,17] based on diffusion flame manifolds is employed, in which different models are used to describe the diffusive transport. In general, flamelet solutions are generated by solving the steady-state flamelet equations with different stoichiometric scalar dissipation rates ranging from thermo-chemical equilibrium to quenching conditions. The chemical source terms are evaluated using the reaction mechanism proposed in [21]. In the current study, the flamelet equations are solved as discussed below assuming a unity Lewis number for the mixture fraction and then the Bilger mixture fraction is evaluated from these results. The mixture fraction is mapped to the Bilger mixture fraction being the first flamelet parameter and the scalar dissipation rate is mapped to progress variable, which becomes the second flamelet parameter.

The laminar flamelet model is a widely-used modeling approach for non-premixed combustion. Originally developed by Peters [18] 30 years ago, it has been extensively validated, modified and extended since. In the present study, we focus on the treatment of differential diffusion and consider the following three approaches:

- (i) Classical steady laminar flamelet using a unity Lewis number assumption [18] (ULNF – unity Lewis number flamelet):
The flamelet equations for temperature T and species mass fractions Y_i read

$$0 = \rho \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} - \frac{1}{c_p} \sum_{i=1}^N \dot{\omega}_i h_i, \quad (1a)$$

$$0 = \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i, \quad (1b)$$

where c_p is the mean specific heat capacity at constant pressure, $\dot{\omega}_i$ is the chemical source term of species i , h_i their

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