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Doubly Conditional Source-term Estimation (DCSE) for the modelling of turbulent stratified V-shaped flame

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ABSTRACT

A partially premixed formulation of Conditional Source-term Estimation including doubly conditioned averages, namely DCSE, is applied to several turbulent stratified V-shaped flames using a Reynolds Averaged Navier Stokes (RANS) approach. Three different stratification levels are considered with different turbulence conditions. In contrast to the authors' initial work (Dovizio et al., 2016), a more elaborate closure of the scalar dissipation rate is implemented in the progress variable variance equation, where a dependence on the local value of the equivalence ratio is considered. Detailed chemistry is included. Good predictions are obtained for the mean axial and transverse velocity components, and progress variable compared to experimental data for the stoichiometric cases, in particular for the lean and rich cases, where the predictions are significantly improved compared to previous numerical studies. The flame thickness is found to be reduced when the stratification increases, consistent with experimental findings. Future work will examine the closure of cross-dissipation terms in the transport equations and the DCSE implementation in LES.

1. Introduction

Lean premixed combustion represents an interesting combustion mode for fossil fuel power generation as it has been shown to provide low emissions and high efficiency, compared to diffusion flames. However, lean premixed flames are more susceptible to combustion instabilities. In order to achieve more stable combustion in fuel lean conditions stratified combustion has provided some good results. In stratified conditions, the flame propagates through non-uniform reactants towards lean mixtures to reduce carbon monoxide (CO) and nitrogen oxide (NO_x) formation [1]. For example, in Direct Injection Spark Ignition (DISI) engines, direct injection of the fuel in the combustion chamber is followed by ignition, while fuel and oxidizer are still mixing. This leads to the reduction of pollutant emissions and fuel consumption due to the spatial stratification of the equivalence ratio [2]. Turbulent stratified flames present some distinct features, different from what is found in premixed flames and have recently been reviewed by Masri [3]. A summary of the experimental findings is presented below.

The introduction of a strong spatial or temporal variation of equivalence ratio has several effects on the flame structure. The three generally accepted and most observed are [4]: (i) variation of flame speed and extension of the flammability limit, (ii) change in the inner structure of the flame, and (iii) dependence of the reaction rate on turbulence and reactive scales. Flame front propagation is higher in the case of turbulent flame with large scale stratification of the equivalence ratio, compared to the corresponding homogeneous mixture at the same mean equivalence ratio [2,5]. This aspect can be related to the fact that heat and radical flux from the richer products supports the leaner flame region, enhancing its resistance to extinction. This characteristic is known as “back support” or “memory effect” [3,5]. Modification of the inner structure of the flame such as wrinkling, curvature and rate of strain is another aspect to be considered in stratified combustion. In particular, wrinkling is due to differential propagation speeds and is enhanced in the stratified case [6–8], in particular if the turbulence is not strong enough to affect completely the flame structure, i.e. the turbulence intensity is comparable with the laminar flame speed: $u'/s_L \approx 1$ (with u' being the fluctuation of the velocity and s_L the laminar flame speed). Sweeney et al. [9], for example, use Line imaging of Raman–Rayleigh scattering and CO-Laser-Induced Fluorescence (LIF) with simultaneous cross-planar OH-Planar Laser-Induced Fluorescence (PLIF) for premixed and stratified low-turbulence methane/air V-flames. The curvature distribution is found to be broader, and flame surface density and scalar dissipation rate are shown to increase in the case of stratified flames. Similar results are obtained in several investigations

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[10–12]. The flame brush thickness is shown to be sensitive to stratification. However, some contradictory results are observed. Several studies report a noticeable increase in flame thickness [8–11] due to stratification, while a decrease of approximately 10% is reported by Robin et al. [4] and negligible change is noted by Bonaldo and Kelman [7]. Further, heterogeneities in equivalence ratio alter the flame curvature as well. Vena et al. [8] observe a slight decrease in curvature for stronger gradients, in contrast to the measurements of Anselmo-Filho et al. [10] and Sweeney et al. [9].

In addition to experimental investigations, several Direct Numerical Simulation (DNS) studies can be found for different stratification conditions and also point out the changes in heat release and burning velocity when a flame propagates through a non-homogeneous mixture [13,14].

Several models for turbulent stratified flames have been proposed in the context of Reynolds Averaged Navier–Stokes (RANS) and Large Eddy Simulation (LES). Common approaches rely on the flamelet concept and describe a stratified flame as a collection of homogeneous premixed flames of different equivalence ratios [15,16]. Thus, the initial turbulent premixed formulation is modified to include the effect of varying mixture fraction values, for example, by changing the chemistry tabulation. This type of model has been shown to work reasonably well when applied to the turbulent stratified flame investigated experimentally by TU Darmstadt [17]. The good performance of these premixed based formulations may be explained by the mild level of stratification in lean conditions. A different flamelet approach may be considered by defining a flamelet transformation that holds in both premixed and non-premixed limiting regimes. This is applied by Knudsen and Pitsch [18] to LES of a lean premixed swirl burner with good predictions in terms of temperature and velocity fields. Nambully et al. also include a sub-grid wrinkling-factor in a Filtered Laminar Flame-Probability Density Function (FLF-PDF) closure to account for different regimes [19], and applied to a stratified bluff-body flame the velocity, mixture fraction and major species are well predicted, while an overprediction of the temperature in the recirculation zone is observed compared to the experiments [20]. A few studies using a flamelet approach are also applied to lean and rich stratified flame regimes [4,21]. Robin et al. [4] present a comparison between their experimental data of stratified turbulent V-shaped flames and numerical RANS results using the Libby-Williams-Poitiers (LW-P) flamelet model. Good agreement with the experiments is noted for the velocity and progress variable profiles in the selected lean stratified flame, but more discrepancies between the numerical predictions and the experimental values appear for the stoichiometric and rich cases. Proch and Kempf perform LES including the Artificially Thickened Flame (ATF) approach with premixed flamelet tabulation applied to the Cambridge/Sandia stratified flames [21]. Turbulent flow field, mean temperature, temperature fluctuation, mean equivalence ratio, equivalence ratio fluctuation and major species mass fractions are well predicted for most regions, some discrepancies with the experimental data being explained by the effect of differential diffusion not included in the simulations. It is interesting to note that in that work, it is concluded that a significant amount of the combustion occurs under quasi premixed conditions due to a negligible equivalence ratio gradient.

In addition to flamelet models, another approach may be considered, Conditional Moment Closure (CMC), which does not rely on the flamelet regime assumption. The derivation of the CMC transport equations does not include any assumption on the flame thickness relative to any turbulent length scale [22]. Thus, in theory, CMC is applicable to any combustion regime. CMC is based on the hypothesis that most of the fluctuations in scalar quantities can be associated with the fluctuations of one or several key quantities, defined as conditioning variables. In the case of non-premixed combustion, the conditioning variable is commonly selected to be mixture fraction, which is a conserved scalar. For premixed combustion, a progress variable may be used [22]. Applications of the CMC approach to stratified configurations have not been presented yet, mainly due to the difficulty of dealing with the conditional scalar dissipation rate closure in premixed regimes [23,24].

In the present work, an alternative method is adopted, Conditional Source-term Estimation (CSE). In the context of numerical simulations of stratified flames, CSE is a good option as it is not restricted to any combustion regime and has been successfully applied to both non-premixed [25–27] and premixed [28,29] flames. In some cases, such as partially premixed or stratified combustion, one conditioning variable is not sufficient. Dovizio et al. [30] have recently extended the singly conditioned CSE formulation to a partially premixed implementation, called Doubly CSE (DCSE). DCSE represents a more advanced closure of the chemical source term and is based on the calculation of doubly conditionally averaged quantities. DCSE is shown to be successful for the simulation of a series of turbulent lifted flames in cold air [30] by using the mixture fraction and a progress variable as conditioning variables. Good predictions are obtained for the lift-off heights and methane concentration, and many aspects of the flame structure are reproduced [30]. Further, DCSE is applied to the Delft-Jet-in-Hot-Coflow (DJHC) flames [31,32], for which two different mixture fractions are defined as conditioning variables. The DJHC flames are well reproduced in terms of velocity, turbulent kinetic energy, temperature and trend of lift-off height decreasing with increasing Reynolds number [31,32]. Recently, CSE and DCSE have been examined for a series of V-shaped premixed and stratified flames, showing good results for the premixed cases and promising predictions for the stratified flames [33]. This previous study is mostly focused on the premixed V-shaped flames and only some initial results of DCSE are presented for the stratified conditions. In particular, in the stratified flame calculations, a simple linear relaxation scalar dissipation rate model is used in the progress variable variance equation, which is shown to be inaccurate, even in premixed conditions, and does not take into consideration the partially premixed configuration. The present investigation builds upon the initial work on stratified V-shaped flames presented in [33].

The objective of the present study is to assess the applicability of DCSE in the context of stratified combustion. In particular, the effect of a more advanced closure for the scalar dissipation rate in the progress variable variance equation is investigated, compared to the previous simplified approach [33]. The partially premixed implementation of DCSE is applied to the study of turbulent stratified V-shaped flames at three different stratification conditions. These are characterized by an equivalence ratio gradient, ranging from a maximum value at the centre of the combustion chamber to a value equal to 0 at the periphery of the domain [4]. An extension of the scalar dissipation model initially proposed by Kolla et al. [34] for premixed conditions to the more general case of partially premixed combustion is introduced. The scalar dissipation rate is related to the heat release rate in premixed conditions and plays an important role in turbulent premixed combustion, appearing as a central quantity in several combustion models [24]. In turbulent premixed flames, the scalar dissipation rate can be defined as the rate of mixing of hot and cold mixtures on the flame surface needed to sustain combustion [24]. It is expected to be equally important for the modelling of stratified flame when a progress variable is considered in the model formulation. The experimental cases simulated are turbulent stratified V-shaped methane–air flames, investigated both numerically and experimentally by Robin et al. [4]. The choice of this set of experiments is motivated by the fact that three levels of stratification are available from lean, stoichiometric and rich combustion regimes, strong equivalence ratio