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Multiple mapping conditioning coupled with an artificially thickened flame model for turbulent premixed combustion

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ABSTRACT

A hybrid Euler/Lagrange approach is introduced for the simulation of turbulent stratified flames. Large eddy simulations (LES) are used for the simulation of the flow field while artificial thickening of the flame provides sufficient resolution for the computation of the evolution of the filtered reaction progress variable. This model is complemented by a sparse Lagrangian particle method that provides instantaneous and local solutions of the species composition and can account for deviations from the flamelet-structure due to turbulence. The combined approach provides a model applicable to different premixed flame regimes including the corrugated and thickened flame regimes. The particle mixing model is based on a multiple mapping conditioning (MMC) approach that conditions mixing on a reference field (the reaction progress variable). Thus, the model ensures localness of mixing in composition space and prevents unphysical mixing of unburnt fluid with burnt fluid across the flame front. The MMC-LES results show good agreement with experimental data, and flamelet-like structures as well as deviations thereof can be predicted. The results are rather insensitive towards the MMC specific modelling parameters but the modelling of the mixing time scale needs to be adapted to achieve consistency between the flame propagation speed predicted by the artificially thickened flame model and the flame dynamics predicted by MMC.

1. Introduction

Lean premixed combustion offers key advantages such as low propensity to soot formation and potentially very low NO_X emissions when compared to other combustion modes such as premixed combustion under stoichiometric conditions or non-premixed combustion. Despite these apparent advantages, lean premixed combustion is not always easy to realize in applications of practical interest as combustion instabilities may occur which leads to the necessity of increasing the fuel concentration locally. In addition, the flows tend to be turbulent and turbulence will interact with the chemistry. This requires rather sophisticated computational models that capture all of the important thermo-physical interactions in the premixed flame. Some common approaches are the modelling of the G-equation [1] or the flame surface density concept [2]. These standard models are of kinematic nature where the flame front is assumed to be thin and effects of finite rate chemistry that may lead to deviations from a laminar flame structure are typically neglected. This is different for the artificially thickened flame (ATF) model [3] where – due to artificially increased diffusion – the flame front is resolved and finite rate chemistry effects can be approximated using reduced [3,4] or tabulated [5] chemical mechanisms. Turbulence-chemistry interactions can be accounted for in even more detail when the joint (velocity and) composition probability density function (PDF) is known [6]. The major advantage of the PDF method is that the chemical source term is closed and no additional approximation needs to be introduced for the modelling of the effects of sub-grid turbulence on the chemical conversion process; thus, the PDF method presents a model that is not confined to a specific combustion regime and can – in principle – be applied to non-premixed, premixed and mixed combustion modes without any major modifications. However, the mixing model, which accounts for the effects of molecular and turbulent diffusion, requires closure, and the

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quality of PDF predictions strongly depends on the accuracy of the mixing model.

Conventional closures such as the interaction by exchange with the mean (IEM), modified Curl's (MC) and the Euclidean minimum spanning tree (EMST) models provided reasonable predictions for premixed flames that burn in the distributed flame regime [7–9]. The application of these models to relatively thin premixed flames, i.e., flames that are within the flamelet regime, is, however, questionable as they allow particles to mix across the flame front. Tirunagari and Pope [10] predicted reasonable flame propagation speeds for LES combined with particle PDF methods without any explicit treatment of the flamelet structure. These encouraging results may be somewhat fortuitous since rather small LES cells were used. A more promising strategy should ensure mixing of particles which are close in composition space as this will prevent (unphysical) mixing of burnt and unburnt fluid across the flame. Haworth [11] coupled the PDF method with premixed laminar flamelet models while Zoller et al. [12] combined the PDF method with the Bray–Moss–Libby-model to locate the flame front and compute a flame surface density, which specifies the probability of a particle to ignite. Both approaches are suitable for the modelling of premixed flames that preserve a flamelet-like structure but do not allow for any deviations thereof. A more universal mixing model that could be applied to all flame regimes would therefore be desirable.

Multiple mapping conditioning (MMC) [13] may represent such a model. The model combines useful features of the PDF method with the basic concepts of a mapping closure for the modelling of the turbulent mixing term. There are deterministic [14] and stochastic [15–17] implementations of the MMC framework in RANS. In the context of LES, Cleary and Klimenko [18] introduced sparse Lagrangian particle methods with a generalised MMC closure for the filtered density function (FDF) that is used to model the LES sub-filter contributions. The expression “sparse” refers to the number of stochastic particles that can be as low as one stochastic particle per 30 LES cells. The MMC mixing model enforces localness of mixing in a (specified) reference space, and it is this conditioning on the reference field that allows for the sparse character of the particle loading. For non-premixed combustion, the LES filtered mixture fraction is defined as such a reference variable and good predictions are obtained for a number of applications [19–21]. The question of finding a suitable reference variable for premixed flames remains open. Sundaram et al. [22,23] discussed the choice of the reference variable in MMC for premixed combustion and suggested a variable similar to the shadow positions introduced by Pope [24]. They successfully demonstrated the effect of their conditioning approach as the flamelet structure of the flame is conserved but its application to realistic burners remains open.

This work does not adopt the strategies suggested by Sundaram and Klimenko [23] but follows more closely the non-premixed MMC approach [18]. The reference variable needs to be adapted for turbulent premixed combustion and we introduce the LES-filtered reaction progress variable as a suitable conditioning variable for sub-grid scale mixing. As the reaction progress variable is not fully resolved on the LES grid, we employ the artificially thickened flame (ATF) approach [3] and approximate the filtered chemical source term using a two-dimensional flamelet generated manifold (FGM) [25]. It is noted here that any flamelet-based model, such as ATF-FGM, does not allow for the prediction of any departures of the flame from the pre-computed composition space as they could be caused by turbulence. In contrast, a stand-alone PDF method may not capture the correct turbulent flame speed but can predict the local thermo-chemical composition of the mixture. The two methods are thus quite complementary and this is why we extend the LES using ATF-FGM by the MMC model. The present study shall demonstrate the general feasibility of a novel premixed flame model that does not require any closure assumptions with respect to the expected flame regime. The premixed flame regime (as indicated by the position of the flame in the Borghi diagram [26]) shall be a model output and its specification shall not be required prior to the simulations.

The specific objective of this study is to demonstrate that the extension of LES-ATF-FGM by MMC

1. is flamelet-consistent despite the sparse character of the particle method
2. can predict possible deviations from the flamelet structure due to turbulence and
3. a suitable set of modelling parameters exists that provides good agreement with experimental data and ensures consistency between the ATF and MMC solutions.

In Section 2, we give a brief summary of the ATF-FGM approach. We then focus on the MMC model and emphasize the differences between the (new) premixed and (existing) non-premixed implementations of MMC. As many industrial applications involve fuel stratification for improved combustion stability, the model is evaluated by comparison with measurements from the Darmstadt turbulent stratified flame (TSF) series [27]. Section 3 introduces the experimental and numerical setups for the flame TSF-A from this series, and the results are presented and discussed in Section 4. Section 5 completes the paper providing a short summary and an outlook for some future work.

2. Theory

The MMC solver is coupled with an LES-ATF-FGM solver and these two approaches are introduced separately in the following two subsections. The final subsection focuses on the coupling of the two solvers within the present work.

2.1. The ATF-FGM model

The ATF-FGM implementation follows the work of Kuenne et al. [5]. In addition to the LES-filtered equations for mass and momentum, the transport equations for the CO_2 mass fraction, $\widetilde{Y}_{CO_2}$, and the mixture fraction, $\tilde{f}$, are solved, where $\tilde{\cdot}$ indicates Favre-filtering. The species composition space is parameterized by mixture fraction (needed to account for the stratification of the flame to be modelled in Section 3) and CO_2 which represents the reaction progress. CO_2 imposes relatively low resolution requirements and presents an adequate choice for lean premixed flames as investigated here. More discussion on suitable definitions of the progress variable can be found in [5]. A pre-computed two-dimensional chemistry table can then be used for the closure of the filtered chemical source term. The table is generated by the FGM method [25] and is based on the GRI-Mech 3.0 reaction scheme [28] using unity Lewis numbers. The unity Lewis number assumption is in line with common practice for modelling this flame [29]. De Swart et al. [30] showed that preferential diffusion of the different species can have opposing effects and cancel each other in methane-air mixtures like those investigated here. An effective Lewis number near unity is a sufficiently accurate approximation. As the LES grid resolution is typically too coarse for resolving the premixed flame front adequately the dynamic artificial thickening procedure [3,31] is applied, i.e., the molecular diffusion is artificially increased by the thickening factor, *F*, such that a desired resolution by approximately 10 LES cells across the flame is ensured. Using ATF, the (thickened) flame is fully resolved on the LES grid and the approach can be coupled with the tabulated FGM