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LES modeling of premixed combustion using a thickened flame approach coupled with FGM tabulated chemistry

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ABSTRACT

Flamelet Generated Manifolds (FGM) tabulated chemistry is used in combination with a thickened flame approach to perform Large Eddy Simulation (LES) of premixed combustion. Two-dimensional manifolds are used to describe the chemistry by the mixture fraction and progress variable. Simulations of one-dimensional flames have been used to verify the coupling of the tabulated chemistry and the LES solver where important features like the grid dependence of flame propagation are carefully addressed. Finally, the method is applied to the turbulent flame of a premixed swirl burner including the complex geometry of the swirl nozzle. Results of the velocity, species and temperature are compared with experimental data. Thereby different efficiency functions are used to show the sensitivity related to this model parameter. Some aspects regarding dynamic thickening, numerical accuracy and computational efficiency are also addressed.

1. Introduction

Lean premixed combustion is of increasing importance in many industrial applications (such as land based gas turbines [1], aero-engines [2] and automotive engines [3]) regarding the pollutant formation due to the lower peak temperature when compared to non-premixed systems. The occurrence of unsteady phenomena like flashback and combustion instabilities makes these flames difficult to control and hence it is desirable to predict their behavior using LES. Since a flammable mixture exists before combustion occurs the flame speed is a decisive parameter and needs to be reproduced by the simulation. This is difficult because the reaction can not be resolved on typical computational grids and models are required to ensure the correct flame propagation. In addition, the model needs to account for the interaction of unresolved vortices with the flame. Therefore the flame speed enters the model as an a priory known parameter, such as in the G-equation or Flame Surface Density concept, or results on its natural way from the integration of the chemical source term. Regarding the latter strategy the use of a filtered chemical look-up table has been proposed very recently by Vreman et al. [4] which has been refined in the F-TACLES (filtered tabulated chemistry for LES) model by Fiorina et al. [5] to allow a proper description of the filtered flame structure and propagation. This approach seems very attractive but not much experience has been gained with it yet. Another well established strategy to resolve the flame on LES meshes is to artificially thicken the flame (Artificially Thickened Flame (ATF)-model).

The ATF-model is very attractive since its theoretical derivation contains no restricting assumptions regarding the flame topology. Due to its universal validity it has been applied to premixed flames [6], lifted flames [7] as well as ignition sequences [8] where finite rate chemistry effects are important. In order to minimize the modeling effort introduced by the modified flame turbulence interaction the thickening factor is limited to resolve the length scales of major species only. Therewith the complexity of the chemical scheme is in general limited to strongly reduced mechanisms (1–3 steps). Of course a small number of reactions is desirable for computational efficiency, but important flame characteristics are difficult to reproduce. As mentioned by Selle et al. [6] and Schmitt et al. [9] especially at higher equivalence ratios errors occur regarding the flame speed and burnt gas temperature. Boudier et al. [10] adjusted the preexponential constant to obtain the correct flame propagation but the burnt gas temperature remained to high in rich regions.

In the present work the ATF concept is combined with a tabulation strategy to include detailed chemistry effects into the LES. Regarding premixed flames two similar tabulation approaches developed simultaneously called FPI (flame prolongation of intrinsic low-dimensional manifolds, ILDM [11]) [12,13] and FGM

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(flamelet generated manifolds) [14,15] proved to be well suited to accurately describe the flame structure and propagation. It will be demonstrated that important flame characteristics can be reproduced over the whole range of equivalence ratios by transporting two controlling variables for mixing (mixture fraction) and reaction progress (CO_2 mass fraction) combined with the FGM table. Compared to reduced mechanisms this method is thought to be a promising alternative when using artificial thickening. Of course more a priori knowledge about the reaction is required when using tabulated chemistry. For example, if heat losses are important that needs to be accounted for by an additional table dimension while it naturally arises in the Arrhenius law of a reduced mechanism. In addition, the freely propagating flame obtained from the one-dimensional detailed chemistry solution is only an approximation for the stretched and curved flame in a turbulent flow field. But this flamelet assumption is not very restrictive as investigated by Poinsot et al. [16] by means of DNS where the domain of flamelet modeling has been found to be much larger than expected from classical combustion diagrams. Further arguments related to the mass burning rate of a stretched and curved flame in combination with the Lewis number are given in Section 2.1.

The outline of this paper is as follows. In Section 2 the chemistry reduction using FGM and the LES solver will be introduced. The coupling of these will be investigated and the quantitative error behavior of flame propagation on coarse grids will be explained by means of theoretical derivations and 1-D numerical simulations. In Section 3 the ATF concept will be summarized and the impact of dynamic thickening based on a flame sensor on the flame turbulence interaction is illustrated. Some interesting findings regarding the numerical treatment of the thickening procedure are also discussed. Finally in Section 4 the model is applied to a methane-air swirl burner at atmospheric pressure where the flame is stabilized by a central recirculation zone which is common practice in gas turbine combustors. To allow for a fully developed turbulent flow the upstream geometry including the bluff-body swirl nozzle of full complexity was included in the computational domain.

2. Coupling of tabulated chemistry with the LES solver

2.1. FGM tabulation

Like many other reduction strategies the technique of flamelet generated manifolds aims at describing detailed chemistry by only a couple of controlling variables. This section is restricted to the manifold construction of a methane-air flame used in this work. A more fundamental description of the theory and its verification can be found in [14,15]. For the table generation, first a one-dimensional freely propagating premixed flame at constant equivalence ratio is simulated using the detailed chemistry one-dimensional flame code Chem1D [17] with the GRI 3.0 reaction scheme [18]. This computation is repeated for different equivalence ratios to span a two-dimensional manifold which can be parameterized by the mixture faction and a reactive scalar as progress variable.

Within this work the non-normalized mass fraction of carbon dioxide is used as progress variable even though it is not strictly monotonic in rich regions ($\phi > 1.2$). In the literature different progress variables (Y_{pv}) built by a linear combination of several (weighted) species mass fractions have been suggested to meet the requirement of being monotonic for all equivalence ratios. Two of them being often used are

$$Y_{pv,1} = Y_{CO_2} + Y_{CO} [19,13] \tag{1}$$

$$Y_{pv,2} = \frac{Y_{CO_2}}{W_{CO_2}} + \frac{Y_{H_2O}}{W_{H_2O}} + \frac{Y_{H_2}}{W_{H_2}} [20,4,21] \tag{2}$$

where W denotes the molar mass of the corresponding species. Unfortunately these progress variables have a much thinner reaction zone compared to Y_{CO2} alone. This is illustrated on the left of Fig. 1 where the thickness of the source term ($\delta(\dot{\omega}_{pv})$) of the different progress variables defined by its full width at half maximum is shown for various equivalence ratios. In the region around stoichiometry the source term of Y_{CO_2} can be resolved using only half of the resolution compared to Eqs. (1) and (2) which is highly desirable. Hence, we decided to neglect the decomposition of CO_2 into CO at high temperature levels by using only the monotonic part of the CO_2 mass fraction to allow for a unique relation to the state variables extracted from the table. The resulting error regarding the prediction of density and temperature defined to be the maximum difference between the value at the turning point of the CO_2 mass fraction (index CO_2,*tp* which is the last monotonic entry) and the correct value obtained in the flamelet behind the turning point

$$\epsilon(\rho) = \frac{\max\left(\rho_{CO_2,tp} - \rho_{flamelet}\right)}{\rho_{CO_2,tp}} \tag{3}$$

is shown on the right of Fig. 1. As one can see $Y_{pv,1}$ and $Y_{pv,2}$ are the more accurate progress variables to describe the complete flame structure for all equivalence ratios while—as expected—deviations from the correct value in the rich region can be observed if Y_{CO_2} is used (the error in flame propagation speed is also below 10%). But this error is small compared to the additional modeling uncertainty introduced by increasing the amount of artificial thickening (see Section 3) to resolve the flame.

The resulting manifold is shown in Fig. 2 where the chemical source term of carbon dioxide is shown as a function of the two controlling variables (equivalence ratio has been used instead of

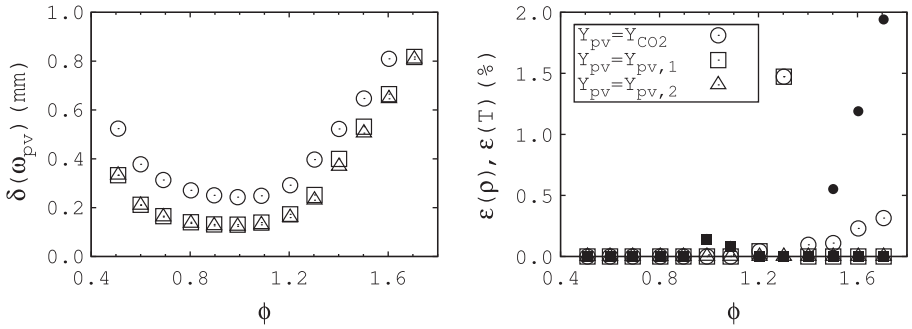

Fig. 1. Evaluation of different progress variables (see Eqs. (1) and (2)) using the results from 1-D simulations of a methane-air flame at $T = 300$ K, $p = 101{,}325$ Pa (GRI 3.0, 300 Gridpoints). Left: Source term thickness. Right: Corresponding error (Eq. (3)) when non-monotonic parts of the progress variable are neglected. Open symbols: error in density ρ, filled symbols: error in temperature T.