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Challenging modeling strategies for LES of non-adiabatic turbulent stratified combustion

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ABSTRACT

Five different low-Mach large eddy simulations are compared to the turbulent stratified flame experiments conducted at the Technical University of Darmstadt (TUD). The simulations were contributed by TUD, the Institute for Combustion Technology (ITV) at Aachen, Lund University (LUND), the EM2C laboratory at Ecole Centrale Paris, and the University of Duisburg-Essen (UDE). Combustion is modeled by a premixed flamelet tabulation with local flame thickening (TUD), a premixed flamelet progress variable approach coupled to a level set method (ITV), a 4-steps mechanism combined with implicit LES (LUND), the F-TACLES model that is based on filtered premixed flamelet tabulation (EM2C), and a flame surface density approach (UDE). An extensive comparison of simulation and experimental data is presented for the first two moments of velocity, temperature, mixture fraction, and major species mass fractions. The importance of heat-losses was assessed by comparing simulations for adiabatic and isothermal boundary conditions at the burner walls. The adiabatic computations predict a flame anchored on the burner lip, while the non-adiabatic simulations show a flame lift-off of one half pilot diameter and a better agreement with experimental evidence for temperature and species concentrations. Most simulations agree on the mean flame brush position, but it is evident that subgrid turbulence must be considered to achieve the correct turbulent flame speed. Qualitative comparisons of instantaneous snapshots of the flame show differences in the size of the resolved flame wrinkling patterns. These differences are (a) caused by the influence of the LES combustion model on the flame dynamics and (b) by the different simulation strategies in terms of grid, inlet condition and numerics. The simulations were conducted with approaches optimized for different objectives, for example low computational cost, or in another case, short turn around.

1. Introduction

The simulation of turbulent combustion has received much attention due to its importance for power generation and transportation. Numerical simulations of applied combustion systems were pioneered in the late seventies in the Reynolds Averaged Navier Stokes (RANS) framework, and 20 years later in the context of Large Eddy Simulation (LES), which resolves the large scale dynamics of a flame.

An LES grid is typically coarser than the thickness of a (stratified) premixed flame and even some of the flame wrinkling patterns. The chemical reaction rates are complex, cover a wide range of time-scales, and lead to a stiff system of equations. As a result, most chemical species cannot be resolved on the meshes that are used for industrial applications, so that subgrid scale modeling is needed for the flame structure and its interactions with the turbulence. A

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recent review of strategies to include combustion chemistry in LES is proposed in [1]. For premixed and stratified combustion, different methods have been developed to capture the propagation of the filtered wrinkled flame fronts, without having to resolve all species contained in the chemical mechanism. Some of these strategies are described below.

A first approach is the Artificial Flame Thickening (ATF) or Thickened Flame Model (TFLES), which artificially thickens the flame front by modifying the diffusion coefficient and the pre-exponential constant [2–4]. This approach is robust and has been applied to complex combustors, using a global chemistry assumption [5]. Detailed chemistry effects can been accounted for by coupling ATF methods with tabulated chemistry techniques for adiabatic [6] and non-adiabatic flames [7].

An alternative is the use of a filter of (at least) the size of the grid spacing. The Flame Surface Density (FSD) concept for LES [8] is based on this idea, which was initially developed for infinitely thin flames and later extended for flames of finite thickness [9]. This strategy has been retained to introduce tabulated chemistry through the Filtered Tabulated Chemistry for LES (F-TACLES) model [10]. The F-TACLES formalism has been developed to capture the filtered flame propagation in complex reactive flow configurations, such as stratified [11] or non-adiabatic flames [12].

Another approach is to solve a smooth scalar field where an iso-surface is defined to represent the instantaneous position of the premixed flame front. This level set or G-equation model has been proposed in the RANS context [13], and was amongst the first model applied to LES [14]. The mathematical formalism of the G-equation has been updated for LES in the corrugated flamelet regime [15] and in the thin reaction zones regime [16,17].

However, one can also apply an LES on a very find grid, with a resolution sufficient to resolve the flame thickness and wrinkling patterns. This results in a Direct Numerical Simulation (DNS) of the flame front, so that no sub-grid model contributions for the reaction rate modeling are needed. The approach is here referred to as "No Combustion Model (NCM)", linked to a (small) detailed reaction mechanism that is solved directly in the LES [18,19]. The method does however require a sufficient grid resolution and a much reduced chemical mechanism without stiff species like CH or HCO.

All these turbulent combustion models have different requirements in terms of grid resolution and numerical scheme. Research groups have therefore developed their own strategies, which involve the combination of the turbulence and combustion models, the numerical schemes, the prescription of boundary conditions, computer hardware, and further choices made by the user. The results of five different strategies are presented and compared in the present paper. The aim of the paper is to illustrate the state of the art in stratified turbulent combustion modeling, as demonstrated for different strategies of different groups. It should be noted that this comparison goes far beyond a comparison of sub-models (e.g. for the reaction source term or for the turbulent flux only), which could be conducted by a single group, but might be affected by a shortcoming in the computational approach. Indeed, the collaboration of five different groups has led to the recognition of certain critical modeling aspects that will be discussed in this paper.

The target for the comparison is the turbulent stratified flame configuration investigated by laser diagnostics at Technische Universität Darmstadt (TUD) [20,21]. This case is strongly influenced by interactions between turbulence, chemistry, heat transfer and fuel/air mixing. It features a relatively simple geometry but encompasses a large range of complex phenomena. Given these advantages and the timely availability of the experimental data, this case was chosen as a target for the TNF workshop, and hence for the comparison presented in the present paper.

Five groups are involved: the Institute of Energy and Power Plant Technology at TUD, the EM2C laboratory at Ecole Centrale Paris (EM2C), the Institute for Combustion Technology (ITV) at RWTH Aachen, Lund University (LUND), and the University of Duisburg-Essen (UDE). All groups employ different flow solvers, which all rely on low Mach number assumptions to achieve an efficient time integration. The TUD applies a premixed flamelet tabulation using ATF, EM2C applies the F-TACLES model, ITV uses a G-equation formalism coupled to a flamelet progress variable approach, LUND describes the combustion chemistry through a 4-steps mechanism combined with NCM, and UDE uses an FSD approach that assumes an infinitely thin flame front.

The simulations differ by the modeling approach, the CFD code, the combustion chemistry, numerical techniques, computational meshes – and other choices made by the user. In spite of these differences, each of these computational strategies is designed to capture the filtered flame propagation speed when subgrid scale flame wrinkling occurs (with the exception of NCM) or when the flame wrinkling is fully resolved. The models account for non-adiabatic effects on the combustion chemistry, so that they are able to capture quenching phenomena induced by heat losses at the burner. As a result, all methods should be able to capture the same global flame properties.

Section 2 gives more details on the turbulent combustion models and their differences and similarities. Section 3 describes the target experiment configuration, and Section 4 presents the different computational setups. The results are then presented and discussed in Section 5.

2. Turbulent combustion models

2.1. Filtered tabulated chemistry for LES (EM2C)

The Filtered Tabulated Chemistry model captures a stratified flame front using the mixture fraction Z and the progress variable Y_c. The mixture fraction Z, equal to 0 and 1 in oxidizer and fuel streams, respectively, captures the fuel-air mixing, whereas the progress variable Y_c (here defined as CO_2 mass fraction) tracks the flame front. The F-TACLES formalism closes the filtered progress variable $\widetilde{Y}_c$ equation in the flamelet regimes [10–12]. The SGS laminar contributions to molecular diffusion and convection and chemical reactions are tabulated by filtering 1-D adiabatic premixed flame elements computed with detailed chemistry and transport. Balance equations for the filtered mixture fraction $\widetilde{Z}$ and the mixture fraction variance $\widetilde{Z}''^2$ [11] are solved in addition to the $\widetilde{Y}_c$ transport equation.

By definition, this model propagates the resolved flame front at the sub-grid scale turbulent flame speed $S_{T,\Delta}$ [11,12]:

$$\rho_0 S_{T,\Delta} = \Xi_\Delta \gamma \int_0^1 \rho_0 S_l{}^{ad}\left(Z'\right) P(Z')\, dZ', \tag{1}$$

In this equation, $S_l{}^{ad}(Z)$ is the consumption speed of a freely propagating adiabatic laminar premixed flame within fresh gases of mixture fraction Z. The sub grid scale flame front wrinkling factor is denoted to by Ξ_Δ.

The mixture fraction Filtered Density Function (FDF) $\widetilde{P}(Z)$ is modeled by a β function characterized by the filtered mixture fraction $\widetilde{Z}$ and the subgrid scale mixture fraction variance $\widetilde{Z}''^2$. The coefficient γ accounts for heat losses [12] and is defined as follows:

$$\gamma = \frac{\int_0^1 \rho_0 S_l\left(Z', \Delta\widetilde{h}\right) P(Z')\, dZ'}{\int_0^1 \rho_0 S_l^{ad}(Z') P(Z')\, dZ'}, \tag{2}$$

The enthalpy defect relative to the fresh gases is defined as $\Delta h = h^{ad}(Z) - h(Z)$, where h is the chemical plus sensible enthalpy and superscript ad refers to adiabatic conditions. The $S_l\left(Z', \Delta\widetilde{h}\right)$ and the laminar consumption speed at a given Δh is estimated from burner-stabilized 1-D flames [22]. In adiabatic flows, γ equals 1 and decreases when heat losses slow down combustion chemistry, to the limit of a quenched flame for $\gamma = 0$.