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LES of turbulent combustion: On the consistency between flame and flow filter scales

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Abstract

A recurrent issue in premixed combustion LES is that the flame thickness is smaller than the grid size. Broadening of the reactive layer is then mandatory to ensure a proper propagation of the filtered flame front. The reactive flow governing equations exhibit then two filter operators of different sizes dedicated to the flow field and the flame front, respectively. The consistency issues between flame and flow filter sizes in LES of turbulent premixed flames are discussed in the present article. A general mathematical formalism considering two different filter sizes is proposed. A new closure of the resulting LES balance equations system is derived in the framework of the Filtered TAbulated Chemistry for LES (F-TACLES) formalism. The new model, called F2-TACLES, is first validated by computing 1-D premixed filtered flames. Then an LES of the complex turbulent premixed PRECCINSTA swirl burner is successfully performed. In particular, the new model formulation improves the prediction of resolved flame/turbulence interactions.

Keywords: Large Eddy Simulation; Turbulent combustion modeling; Turbulent premixed flames; Tabulated chemistry

1. Introduction

An efficient modeling approach for Large Eddy Simulation (LES) of turbulent premixed combustion is to identify the flame front as a propagating surface. The G-equation formalism tracks this surface assumed infinitely thin using level-set numerical techniques [1–4]. Despite a simplified description of the chemical processes, this approach is commonly used in LES of premixed combustion [1,3–5].

Infinitely thin surface approaches however remain limited as they do not describe the inner flame structure. Accounting for the flame thickness is necessary to access thermochemical variables within the flame front but raises several issues in LES of premixed combustion. Figure 1 illustrates the propagation of a filtered flame front in a turbulent environment, using a mesh grid of size Δ_x. According to [6], the velocity field $\widetilde{\mathbf{u}}$, Favre-filtered by a Gaussian function of width

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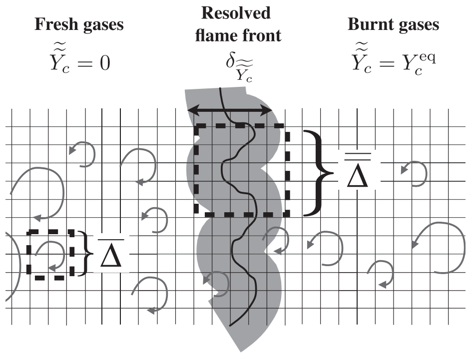

Fig. 1. Filter size issues in turbulent combustion LES.

$\overline{\Delta}$, is well resolved on the LES grid when the resolution criteria $\overline{\Delta} > 2\Delta_x$ is satisfied. The flame is here modeled by a progress variable Y_c, monotonically increasing from 0 in the fresh gases to Y_c^{eq} in the burnt gases. In practical meshes, the flame thickness, defined as $\delta_{Y_c} = Y_c^{eq}/max(|\nabla Y_c|)$, is thinner than the mesh size Δ_x [7,8]. Therefore, filtering the progress variable field at the width $\overline{\Delta}$ introduces a resolved flame front of thickness $\delta_{\widetilde{Y}_c} \approx \overline{\Delta}$ with $\overline{\Delta} \approx 3\Delta_x$. As further illustrated in Section 2.1, the chemical reaction layer is then under-resolved inducing a misprediction of the flame propagation speed [9,10].

Two major alternatives are then possible to capture both the flame propagation and the flame structure. The first is to artificially thicken the flame front (Thickened Flame model for LES) and to model sub-grid scale (SGS) wrinkling [11]. Efficient and robust, the TFLES model can be combined either with simple [12] or tabulated chemistry [10,13] formalisms. An alternative is to introduce a filter of size $\overline{\overline{\Delta}} > \overline{\Delta}$ dedicated to the flame front. Initially developed for infinitely thin flame front and for single-step chemistry [14–16], this strategy has recently been extended to tabulated chemistry by the Filtered Tabulated Chemistry for LES (F-TACLES) model [9,17]. Simulations of propagating filtered premixed planar flames show that the flame resolution criterion $\overline{\overline{\Delta}}/\Delta_x$ depends on numerical conditions [18]. For instance, the criteria $\overline{\overline{\Delta}}/\Delta_x \geqslant 8$ is required in [9] to predict the proper propagation speed of a laminar premixed filtered flame.

Filtering both flow and thermochemical variables at a unique scale $\overline{\overline{\Delta}}$ would not take full benefit of the grid resolution out of the reaction layer. Therefore, turbulent premixed combustion LES involves, implicitly or explicitly, two filter operators of size $\overline{\overline{\Delta}}$ and $\bar{\Delta}$. The condition $\overline{\overline{\Delta}} > \bar{\Delta}$ is fulfilled in practical combustion LES. The influence of two different filter operators on a combustion LES mathematical formalism has never been studied to our knowledge. The mathematical formalism of the general problem is first developed. Two different strategies to treat differences between flame and flow filters are then proposed in the framework of the F-TACLES model. Both model formulations are then tested on the LES of a swirling premixed flame for which experiments [19] and Direct Numerical Simulations [20] are available.

2. Two-scales filtering in turbulent combustion LES

2.1. Problem formalism

$\overline{\Phi}$ and $\widetilde{\Phi}$ denote the Reynolds and Favre filtering of a variable Φ at size $\overline{\Delta}$ while $\overline{\overline{\Phi}}$ and $\widetilde{\widetilde{\Phi}}$ are defined as the values of Φ filtered at size $\overline{\overline{\Delta}}$. Filtering continuity and momentum equations at the filter scale $\overline{\Delta}$ leads to the following system:

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho}\tilde{\mathbf{u}}) = 0 \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\rho}\tilde{\mathbf{u}}\tilde{\mathbf{u}}) = -\nabla \overline{P} + \nabla \cdot (\bar{\tau} + \bar{\tau}^t) \tag{2}$$

where $\bar{\rho}$ and $\tilde{\mathbf{u}}$ are the filtered density and velocity vector, respectively. $\bar{\tau}$ is the filtered viscous tensor and $\bar{\tau}^t = -\bar{\rho}(\widetilde{\mathbf{u}\mathbf{u}} - \tilde{\mathbf{u}}\tilde{\mathbf{u}})$ the Reynolds stresses. In a low-Mach number context, P denotes the hydrodynamic pressure.

Considering reactive flows, the propagation of a flame front is governed by the chemical species balance equation:

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_k) = -\nabla \cdot (\rho Y_k V_k) + \rho \dot{\omega}_{Y_k} \tag{3}$$

where $Y_k, \dot{\omega}_{Y_k}$ and V_k are the mass fraction, the chemical reaction rate and the molecular diffusion velocity of the k-th species, respectively. Assuming steady state in the flame coordinate system, the integration of Eq. 3 in the direction x_n normal to the flame front gives the flame consumption speed S_l:

$$S_l = \frac{1}{\rho^u (Y_k^b - Y_k^u)} \int_{-\infty}^{+\infty} \rho \dot{\omega}_{Y_k} dx_n \tag{4}$$

where superscripts u and b refer to fresh and burnt gases states, respectively. Equation (4) shows that a reliable computation of the flame surface propagation requires a fine numerical resolution of the chemical reaction rate $\dot{\omega}_{Y_k}$ involved in the integral of the RHS. This issue is illustrated in Fig. 2 showing the CO_2 chemical reaction rate $\rho\dot{\omega}_{Y_{CO_2}}$ normalized by its maximum value and extracted from a 1-D laminar premixed CH_4–air flame computed using a detailed chemical scheme [21]. This