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Filtered Tabulated Chemistry for non-premixed flames

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Abstract

The objective of the present study is to design a modeling strategy for LES of laminar diffusion flame regimes, *i.e.* without SGS wrinkling. A non-premixed model dedicated to capture unresolved laminar flame structure is then proposed. For that purpose, the Filtered Tabulated Chemistry for Large Eddy Simulation is adapted to diffusion flames. A filtered look-up table computed from a collection of strained 1-D counterflow flames is generated. The filtered flame structure and thickness is captured with three controlling variables which are the filtered mixture fraction, the filtered progress variable and the filter size. This approach is successfully applied to 1-D and 2-D unresolved counter-flow flame simulations. The filter size governs the minimal thickness of the filtered thermal layer.

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Keywords: Non-premixed combustion modeling; Tabulated chemistry; Laminar flames; Large-Eddy Simulation

1. Introduction

Numerous non-premixed combustion LES models rely on a statistical description of flame turbulence interactions [1]. Commonly used approaches to estimate subgrid Filtered Density Function (FDF) are based on probability transport equations [2], Condition Moment Closure [3,4] or presumed FDF [5,6]. These approaches are performing well in the presence of high level of turbulent wrinkling but do not guarantee that the proper flame structure is recovered when the wrinkling is fully resolved or in laminar cases.

This situation is for instance encountered in the simulation of liquid rocket engines, that operates at very high pressures, typically around 10 MPa. Indeed, experimental investigations have shown that the coaxial injection system promotes the development of a turbulent non-premixed jet flame anchored at the injector lips [7,8]. Direct numerical simulation of this near-burner region show that the flame front is very thin (of the order of 10–100 μm) and weakly wrinkled by turbulent motions [9,10]. Because of numerical resolution issues, Large Eddy Simulation of such flame regime is extremely challenging. This is illustrated in Fig. 1, which shows a schematic view of a developing turbulent reactive mixing layer behind a splitter plate. At the flame basis, the flame thickness $\delta_Z^0 = 1/\max|\nabla Z|$, where Z is the mixture fraction, is much thinner than the LES grid size used in practical configuration.

The objective of the present study is to discuss modeling issues in LES of laminar diffusion flame regimes, *i.e.* when no flame wrinkling occurs at the Sub Grid Scale (SGS). A modeling strategy, which controls the filtered flame thickness on unresolved situations *i.e.* when the flame thickness is smaller

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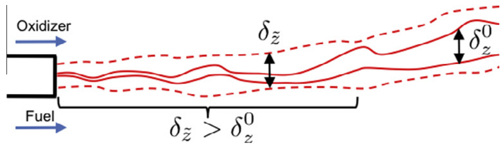

Fig. 1. Schematic representation of a diffusion flame stabilization behind a splitter plate. The continuous line represents the unfiltered flame brush, while the dashed line shows the filtered flame that is required to be properly handled by a LES mesh. δ_z^0 is the flame thickness and $\delta_{\tilde{z}}$ is the filtered flame thickness.

than the grid size, is proposed. In Section 2, the structure of a filtered non-premixed flame front is analyzed by post-processing a collection of 1-D filtered counterflow detailed chemistry flames. In Section 3, a combustion model is developed in the framework of the Filtered Tabulated Chemistry model for LES (F-TACLES), initially developed for premixed [11] and stratified [12] combustion. In Section 4, the model is implemented in a 1-D Low Mach number counter-flow solver and in a multi-dimensional compressible flow solver. Numerical simulations of filtered (unresolved) diffusion flames are presented.

2. The chemical structure of a filtered laminar diffusion flame

2.1. Conservation equations and numerical configuration

The chemical structure of non-premixed combustion is investigated on 1-D counterflow flame configurations, governed by the following set of balance equations [13]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_n}{\partial x_n} + 2\epsilon\rho U = 0 \tag{1}$$

$$\rho\frac{\partial U}{\partial t} + \rho u_n \frac{\partial U}{\partial x_n} - \epsilon(\rho U^2 - \rho_\infty) = \frac{\partial}{\partial x_n}\left(\mu\frac{\partial U}{\partial x_n}\right) \tag{2}$$

$$\rho\frac{\partial Y_k}{\partial t} + \rho u_n \frac{\partial Y_k}{\partial x_n} = -\frac{\partial \rho V_k Y_k}{\partial x_n} + \dot{\omega}_k \tag{3}$$

$$\rho c_p\frac{\partial T}{\partial t} + \rho c_p u_n \frac{\partial T}{\partial x_n} = \frac{\partial}{\partial x_n}\left(\lambda\frac{\partial T}{\partial x_n}\right) - \left(\rho\sum_{k=1}^{k=N_{sp}} c_{p,k} Y_k V_k\right)\frac{\partial T}{\partial x_n} - \sum_{k=1}^{k=N_{sp}} h_k\dot{\omega}_k \tag{4}$$

where x_t and x_n are the spatial coordinates in the direction parallel and normal to the flame front, respectively. $U(x_n) = u_t/\epsilon x_t$, where ϵ is the strain rate and u_n and u_t are the velocities normal and parallel to the flame front, respectively. Y_k and $\dot{\omega}_k$ are the species mass fraction and chemical mass reaction rate of kth species, respectively. T is the temperature, ρ is the density, c_p is the mixture heat capacity, h_k is the enthalpy per unit of mass of species k and $V_k Y_k = -D_k \partial Y_k/\partial x_n$ with D_k the diffusion coefficient of species k. Thermochemical quantities are computed using GRI 3.0 detailed chemistry scheme [14] which involves 53 species and 325 elementary reactions.

To highlight the influence of filtering on diffusion flames, pure methane and pure oxygen ($p = 101\,325$ Pa, $T_{inj,O_2} = T_{inj,CH_4} = 300$ K) one-dimensional counterflow diffusion flames are computed for various strain rates ϵ. Calculations are done under unity Lewis number assumption.

2.2. Filtered counter-flow diffusion flames

Figure 2 plots the mixture fraction Z (equal to 0 and 1 in the oxidizer and fuel streams, respectively) and temperature T of the counterflow CH_4/O_2 flame configuration as a function of x_n for two different strain rates: $\epsilon = 1000\ s^{-1}$ and $\epsilon = 10\,000\ s^{-1}$. The corresponding resolved flame thicknesses $\delta_Z = 1/\max(|\nabla Z|)$ are 1.09 mm and 0.34 mm, respectively.

To mimic LES conditions, mixture fraction and flow thermo-chemical variables solutions are spatially filtered using a gaussian filter operator of width $\Delta = 1$ mm. Filtered flame solutions are superimposed in Fig. 2. Resulting filtered flame thicknesses $\delta_{\overline{Z}} = 1/\max(|\nabla\overline{Z}|)$ equal 1.47 mm for $\epsilon = 1000\ s^{-1}$ and 0.86 mm for $10\,000\ s^{-1}$.

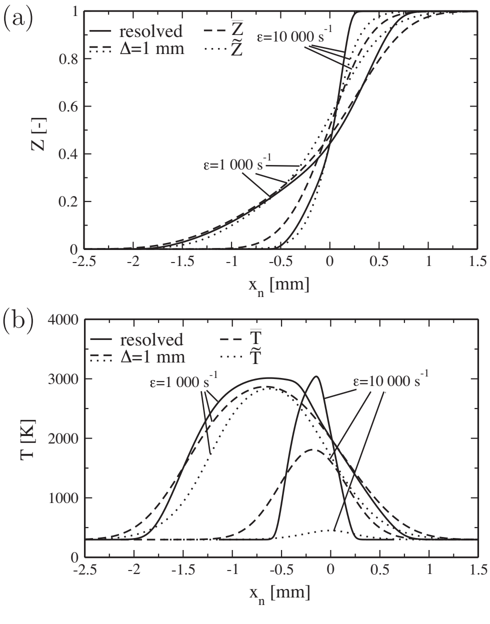

Fig. 2. *Impact of filtering on the flame structure* (a) Mixture fraction Z and (b) temperature T of a counter flow diffusion flame for strain rates ϵ=1000 s^{-1} and 10 000 s^{-1}. Resolved flames and filtered flames with filter size $\Delta = 1$ mm are shown.

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