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The influence of combustion SGS submodels on the resolved flame propagation. Application to the LES of the Cambridge stratified flames

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Abstract

In Large Eddy Simulation (LES) of premixed and stratified combustion, the overall prediction of the flame consumption speed depends on various subgrid scale (SGS) submodels such as the flame wrinkling, the fuel stratification or heat losses. The objective of this study is to investigate the LES sensitivity to the submodeling strategies. Different heat losses and SGS flame wrinkling models are presented in the context of the Filtered TAbulated Chemistry for LES (F-TACLES) formulation. LES of the non-adiabatic non-swirling bluff-body stabilized Cambridge flames (SwB burner) are presented. In this complex configuration, both flame brush and flow dynamics are influenced by flame consumption speed submodels. First, accounting for heat losses impacts the prediction of both velocity and temperature of the inner recirculation zone (IRZ). Second, model constants involved into SGS wrinkling submodels have a great impact on the mean flame brush position. The non-adiabatic formulation combined with a dynamic estimation of the SGS wrinkling model constant appears to be a very attractive approach and gives a very good prediction of both the mean flame location and the IRZ flow dynamics.

Keywords: Large Eddy Simulation; Turbulent stratified combustion; Heat losses; SGS wrinkling model; Dynamic modeling

1. Introduction

Large Eddy Simulation of turbulent reactive flows is an attractive strategy to capture unsteady phenomena governing combustion dynamics and flame stabilization mechanisms. A first modeling approach is to describe the flame front as a propagating infinitely thin surface (G-equation formalism [1]). A second possibility consists in handling the flame thickness resolution using thickening [2,3] or spatial filtering [4,5] formalisms. These strategies differ in the chemical flame structure description, but all require the modeling of the subgrid scale turbulent flame consumption speed [6], which is strongly influenced by subgrid scale

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complex interactions between turbulence, chemistry, heat transfer and mixing. These phenomena are captured by dedicated submodels but their combined influences on the aerodynamic and flame brush predictions have not been investigated yet. The objective of this work is to assess the overall sensitivity of the reactive flow dynamics to the assumptions made to design these submodels.

Our study is conducted through several simulations of the non-swirling non-adiabatic stratified burner SwB [7], experimentally investigated at Cambridge University and at Sandia National Laboratories. Experimental campaigns reveal that the flame structure is influenced by fuel stratification, turbulence, heat losses and differential diffusion. The first part of this article describes the turbulent combustion model, named Filtered TAbulated Chemistry for LES (F-TACLES) [5,8,9] and retained here for the numerical investigations. Submodels influencing the prediction of the subfilter flame consumption speed are discussed. The second part of the article presents a LES parametric study of the SwB configuration. The impact of heat losses on the flame stabilization process and temperature is discussed. Then, a sensitivity analysis is conducted to assess the influence of subgrid scale wrinkling modeling on the mean flame brush and flow dynamics predictions.

2. Combustion model

2.1. Closure of the progress variable filtered equation

In stratified combustion, the flame front is captured by the mixture fraction z and the progress variable Y_c. Mixture fraction z, equal to 0 and 1 in oxidizer and fuel streams, respectively, is used to capture the fuel–air mixing. Progress variable Y_c, equal to 0 and $Y_c^{eq}(z)$ in fresh and burnt gases, respectively, tracks the flame front. The F-TACLES formulation closes the filtered progress variable $\widetilde{Y}_c$ equation in flamelet regimes as [5,8,9]:

$$\frac{\partial \bar{\rho}\widetilde{Y_c}}{\partial t} + \nabla\cdot(\bar{\rho}\widetilde{\mathbf{u}}\widetilde{Y_c}) = \nabla\cdot\left(\Xi_\Delta\gamma\alpha_{Y_c}^{Tab}\rho_0 D_0\nabla\widetilde{Y_c}\right) - \Xi_\Delta\gamma\left(\Omega_{Y_c}^{Tab} + \bar{\rho}\widetilde{\omega}_{Y_c}^{Tab}\right) \quad (1)$$

where ρ and $\mathbf{u}$ are the flow density and velocity, respectively. Subscript 0 denotes reference quantities. By construction, this model propagates the resolved flame front at the subgrid scale turbulent flame speed $S_{T,\Delta}$ [8,9]:

$$\rho_0 S_{T,\Delta} = \Xi_\Delta\gamma\int_0^1 \rho_0 S_l^{ad}(z')P(z')\,dz' \quad (2)$$

where $S_l^{ad}(z)$ is the consumption speed [6] of a freely propagating adiabatic laminar premixed flame within fresh gases of mixture fraction z, Ξ_Δ the flame front wrinkling factor, measuring the subgrid scale flame surface and γ a coefficient accounting for heat losses [9]. In the following, the mixture fraction Filtered Density Function (FDF) $P(z)$ 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 functions $\alpha_{Y_c}^{Tab}, \Omega_{Y_c}^{Tab}$ and $\widetilde{\omega}_{Y_c}^{Tab}$ in Eq. (1) are designed to model the unresolved contributions to molecular diffusion, convection and chemical reaction, respectively. They are tabulated by filtering 1-D adiabatic premixed flame elements computed including detailed chemistry and complex transport and stored as a function of four parameters: $\widetilde{Y}_c, \widetilde{z}, \widetilde{z''^2}$ and the filter scale Δ [8,9]. Δ is chosen so that the reaction layer thickness (based on $\widetilde{\omega}_{Y_c}^{Tab}$) is resolved on a minimum of 4 nodes [10] leading to $\Delta \approx 5\Delta_x$ where Δ_x denotes the cell size. Balance equations for the filtered mixture fraction $\widetilde{z}$ and the mixture fraction variance $\widetilde{z''^2}$ [8] are solved in addition to the $\widetilde{Y}_c$ balance equation.

2.2. Modeling dependencies of $S_{T,\Delta}$

Equation (2) evidences that modeling choices for Ξ_Δ, γ and $P(z')$ directly influence the flame consumption speed. The role of $P(z')$ was discussed previously [8] and the present work focusses on the modeling of the subgrid scale flame wrinkling Ξ_Δ and the heat loss correction γ factors.

2.2.1. Modeling the influence of heat losses

The impact of heat losses is accounted for through the correction factor γ modeled as [9]:

$$\gamma = \frac{\int_0^1 \rho_0 S_l\left(z', \Delta\widetilde{h}\right)P(z')\,dz'}{\int_0^1 \rho_0 S_l^{ad}(z')P(z')\,dz'} \quad (3)$$

where $\Delta\widetilde{h}$, the enthalpy defect relative to the fresh gases, is defined as $\Delta\widetilde{h} = h^{ad}(\widetilde{z}) - \widetilde{h}$. h^{ad} denotes the adiabatic (sensible plus chemical) enthalpy and only depends on mixture fraction and fresh gas temperature while $\widetilde{h}$ is the resolved enthalpy accounting for heat loss. $S_l\left(z', \Delta\widetilde{h}\right)$, the laminar consumption speed at a given Δh, is estimated from burner-stabilized 1-D flames [11]. The heat loss correction factor γ is computed from both the 1-D non-adiabatic flame thermochemical structure and the mixture fraction FDF and does not necessitate any ad hoc parametrization. $\gamma = 1$ in adiabatic flows and decreases when heat losses slow down the combustion chemistry. The limit $\gamma = 0$ corresponds to flame quenching.

2.2.2. Modeling the subgrid scale flame wrinkling

The subgrid scale flame wrinkling model is based on the expression initially proposed by Charlette et al. [12] and later improved [13]: