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A posteriori tests of a dynamic thickened flame model for large eddy simulations of turbulent premixed combustion

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ABSTRACT

Dynamic models where model parameters are automatically adjusted from known resolved fields are a very attractive formulation for large eddy simulations. Now widely used for unresolved momentum transport, this approach remains rather marginal to describe filtered reaction rates despite of very promising results. Global and local dynamic formulations for the flame wrinkling factor are combined with the Thickened Flame (TFLES) model to simulate the F3 pilot stabilized jet flame studied experimentally by Chen and coworkers. The influence of physical (flame wrinkling inner cut-off length scale) and numerical (test filter width, averaging procedure, updating frequency) characteristics of a flame wrinkling factor dynamic model for turbulent premixed combustion is investigated. Numerical results are discussed in terms of mean flow fields as well as dynamical behaviors. It is shown that the dynamic model is robust and relatively insensitive to the numerical input coefficients to be provided beforehand in the code. This finding indicates that the model parameter does not need to be adjusted any more. However, a model for the inner cut-off scale of flame wrinkles, lost in the filtering process, is required.

1. Introduction

Progress in gas turbines or automotive engines is directly linked to the capacity of computational fluid dynamics (CFD) tools to predict correctly the behavior of these complex systems. Large eddy simulation (LES) is now routinely used to improve the design of such combustion devices [1–3]. In LES, the largest structures of the flow are captured by the grid while the effects of the small ones are modeled.

One of the challenges in combustion problems of large eddy simulations is the fact that the flame front is too thin to be resolved on the computational mesh. To overcome this difficulty, several approaches have been developed. Examples include flame front tracking techniques, such as the G equation [4,5], the use of filters larger than the mesh size [3,6] and the TFLES approach in which diffusion and pre-exponential factors are modified in order to artificially thicken the flame [7–9]. This last strategy is adopted in this work.

Another major topic that draws attention is the modeling of the sub-grid terms that appear in filtered balance equations. Thus, unresolved flame/turbulence interaction is a crucial point and a good model for the sub-grid turbulent flame speed [1,3], directly related to the flame front wrinkling factor [8,9], or to the sub-grid scale flame surface density [6] is mandatory. However, usual algebraic models assume equilibrium between turbulence motions and flame surface and consequently they cannot handle transient situations [10]. This is the case of a flame kernel growth or even a jet flame initially laminar during the early stages of the flame development and then progressively wrinkled by turbulence motions. One way to overcome this problem is to solve a balance equation for the filtered surface density [10,11] or for the wrinkling factor [12] but new unclosed terms appear.

An alternative is to develop dynamic combustion models. Dynamic modeling is based on the filtering of the instantaneous resolved fields at a test filter scale larger than the original LES filter. The model is then assumed to hold at both scales and the model parameter can be obtained by solving a “Germano-like” equation [13]. This strategy has been successfully applied by Charlette et al. [14] and Wang et al. [15] in the context of the TFLES model. Charlette et al. [14] carried out 3D simulations of premixed flames in decaying isotropic turbulence and comparisons between DNS and LES showed that the dynamic procedure allows the LES to reproduce the total reaction rate of the DNS quite well. Wang et al. [15] improved the procedure and simulated the turbulent Bunsen flames studied experimentally by Chen et al. [16] over three different operating conditions and results were in good agreement with the experimental data.

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In the Flame Surface Density (FSD) context, Knikker et al. [17,18] proposed a model based on a fractal analysis [19,20] and a similarity assumption [21]. The model was validated *a priori* from experimental data obtained by *OH*-radical laser induced fluorescence in a turbulent premixed propane/air flame. Gubba et al. [22] retained this approach to investigate the propagation of a turbulent premixed flame through obstacles in a laboratory scale combustion chamber. Wang et al. [23] implemented a dynamic version of Boger et al. [6] flame surface density algebraic model to reproduce the growth of a flame kernel in a homogeneous and isotropic turbulent flow field. Two- and three-dimensional simulations were carried out and results were compared with the experimental data from Renou [24].

Im et al. [25] and Knudsen and Pitsch [26] also developed dynamic models in the G-equation framework. Im et al. [25] tested their model in a forced homogeneous and isotropic turbulence case, while Knudsen and Pitsch [26] chose the F3 jet flame investigated experimentally by Chen et al. [16].

More recently, dynamical modeling has also been combined with tabulated chemistry techniques [27]. Schmitt et al. [28] obtained very good preliminary results for the Tecflam burner configuration [29,30] using a dynamic local formulation. Mercier et al. [31] simulated the Cambridge stratified swirl burner (SwB) [32,33] using different heat losses and SGS flame wrinkling models, including the dynamic formulation.

Other authors applied the dynamic formalism to compute variances and scalar dissipation rates of a mixture fraction, that enter non-premixed combustion models [34–38]. These procedures can be denoted “indirect approaches”, to differ from the previous ones that involves directly the reaction rate term.

However, many points remain unclear and not yet investigated, in particular the influence of physical (flame wrinkling inner cut-off length scale) and numerical (test filter width, averaging procedure, updating frequency) characteristics of the model. In the present paper, global and local formulations [39,40] are analyzed in the framework of the TFLES model. In the next section, the basic concepts of the TFLES combustion model are briefly discussed and the dynamic procedure is presented based on the previous *a priori* and *a posteriori* works [14,15,39–41]. Subsequently, the turbulent jet flame configuration investigated by Chen et al. [16] is described together with computational details. Global and local saturated formulations are analyzed as well as the influence of the model coefficients that must be specified beforehand in the code. Conclusions are drawn.

2. Modeling

2.1. The thickened flame model (TFLES)

Flames are artificially thickened to be resolved on numerical grids by multiplying diffusion and dividing reaction rates by a thickening factor $\mathcal{F}$. The modified flame front of thickness $\mathcal{F}\delta_L^0$ propagates at the same laminar flame speed s_L^0 as the original flame of thickness δ_L^0 [7,42]. However, when the flame is thickened, the interaction between turbulence and chemistry is modified and the flame becomes less sensitive to turbulence motions [8]. An efficiency function has been derived to counteract this effect by increasing the flame propagation velocity [8,9]. Charlette et al. [9] introduce a sub-grid scale wrinkling factor, Ξ_Δ that measures the ratio of the total flame surface to the resolved flame surface in the filter volume and directly related to the sub-grid scale flame surface lost because of the thickening process. The balance equations for filtered species mass fractions $\widetilde{Y}_k$ are written as:

$$\frac{\partial \overline{\rho}\widetilde{Y}_k}{\partial x} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Y}_k) = -\nabla \cdot (\Xi_\Delta \mathcal{F} \overline{\rho \mathbf{V}_k} \widetilde{Y}_k) + \frac{\Xi_\Delta}{\mathcal{F}} \dot{\omega}_k(\widetilde{Q}) \tag{1}$$

where ρ is the density, $\mathbf{u}$ the velocity vector, $\mathbf{V_k}$ the diffusion velocity of species k, expressed here using the Hirschfelder and Curtiss approximation [3,43] and $\dot{\omega}_k$ the reaction rate of species k, estimated from Arrhenius law. Q denotes any quantity entering the computation of the reaction rate, such as species mass fractions or temperature. $\overline{Q}$ and $\widetilde{Q}$ denotes filtered and mass-weighted filtered quantities, respectively ($\overline{\rho}\widetilde{Q} = \overline{\rho Q}$). By construction, Eq. (1) propagates a flame front of thickness $\mathcal{F}\delta_L^0$ at the sub-grid scale turbulent flame speed $\Xi_\Delta s_L^0$. Charlette et al. [9] modeled the wrinkling factor with a power-law relationship. Wang et al. [15] slightly modified the initial expression and wrote:

$$\Xi_\Delta = \left(1 + \min\left[\frac{\Delta}{\delta_c} - 1, \Gamma_\Delta\left(\frac{\Delta}{\delta_L^0}, \frac{u'_\Delta}{s_L^0}, Re_\Delta\right)\frac{u'_\Delta}{s_L^0}\right]\right)^\beta \tag{2}$$

δ_c is the inner cut-off length scale (i.e. the smallest scale for the interaction of turbulent eddies with the premixed flame front) assumed equal to the laminar flame thickness δ_L^0. The efficiency function Γ_Δ measures the ability of vortices to effectively wrinkle the flame front, u'_Δ and $Re_\Delta = u'_\Delta \Delta/\nu$ are the sub-grid scale turbulence intensity and Reynolds number, respectively, ν being the fresh gas kinematic viscosity. β is the model parameter to be specified.

However, direct numerical simulations [39,40] showed that Eq. (2) is often saturated, i.e. the minimum term is usually controlled by the $(\Delta/\delta_c - 1)$ contribution. Therefore, Eq. (2) reduces to:

$$\Xi_\Delta = \left(\frac{\Delta}{\delta_c}\right)^\beta \tag{3}$$

Eq. (3) corresponds to a fractal model [19,20,44], where $D = \beta + 2$ is the fractal dimension of the flame surface. Note that this expression no longer requires the modeling of the sub-grid scale turbulence intensity, u'_Δ. However, a constant fractal dimension would correspond to a uniform wrinkling factor over the flow field which is generally not verified. In fact, Eq. (3) with space and time dependent dynamic β values is more general than a usual fractal model and the saturated form of Eq. (2) as this equation is easily recast as:

$$\Xi_\Delta = \left(\frac{\Delta}{\delta_c}\right)^{\beta'} \tag{4}$$

with

$$\beta' = \beta \frac{\log\left(1 + \min\left[\frac{\Delta}{\delta_c} - 1, \Gamma_\Delta\left(\frac{\Delta}{\delta_L^0}, \frac{u'_\Delta}{s_L^0}, Re_\Delta\right)\frac{u'_\Delta}{s_L^0}\right]\right)}{\log\left(\frac{\Delta}{\delta_c}\right)} \tag{5}$$

The thickened flame model is retained in this work that focuses on the dynamic determination of the flame wrinkling factor Ξ_Δ. This wrinkling factor enters also other models such as algebraic flame surface density [6] or F-TACLES [27]. All these models will provide similar results at least as long as the flamelet assumption holds, as confirmed in practice.

2.2. Dynamic formulation

The exponent β of the power law model given by Eq. (3) can be estimated dynamically following a Germano-like procedure. The principle is to compare the progress variable source term computed from test-filtered variables and the test filtered progress variable source term [14,15]. The procedure may also be applied in terms of flame surfaces [23,39–41], writing the filtered progress variable reaction rate as [45]:

$$\overline{\dot{\omega}}_c = \rho_u s_L^0 \Sigma \tag{6}$$