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Large eddy simulation of a turbulent swirling premixed flame coupling the TFLES model with a dynamic wrinkling formulation

Pedro S. Volpiani, Thomas Schmitt, Denis Veynante*

Laboratoire EM2C, CNRS/Ecole CentraleSupélec, Université Paris-Saclay, Grande Voie des Vignes, 92295 Chatenay-Malabry, France

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ABSTRACT

Dynamic models that take advantage of the known resolved scales to automatically adjust the model parameters have proved to be very effective in large eddy simulations (LES). Global (uniform parameter evolving only with time) and local (parameter evolving both in space and time) dynamic formulations for the flame wrinkling factor are combined with the Thickened Flame (TFLES) model and simulations of the semi-industrial PRECCINSTA burner studied experimentally by Meier et al. (2007) are performed for the stable and unstable configurations. The global formulation predicts a time-dependent model exponent that remains close to 0.5 for the stable flame and oscillates strongly around 0.8 for the pulsating flame. The local formulation adapts the model parameter locally and automatically damps the wrinkling factor in the vicinity of walls, contrary to the global formulation requiring a wall law. The usual non-dynamic approach with an appropriate parameter is found to capture flow statistics of the stable flame with good accuracy, both in terms of Favre and quasi-Reynolds averages. However, the self-excited mode of the pulsating flame is predicted only with the dynamic formalism. The fractal dimension of the unstable flame is found to vary locally and depends on the phase within the period of oscillation. Dynamic models may then play an important role in the prediction of combustion instabilities.

1. Introduction

Dynamic models have proved to be a powerful tool in Large Eddy Simulations (LES). The basic idea of such models, developed to describe sub-grid scale momentum transport [2], is to take advantage of the known instantaneous resolved large scales to automatically adjust model parameters. The instantaneous resolved field is filtered at a test filter scale larger than the original LES filter. The model is then assumed to hold at both scales and model parameters are solutions of a Germano-like equation.

While dynamic models are now routinely used for momentum transport, their application to reaction rate modeling in combusting flows remains rather scarce and often restricted to simple flow configurations (flame embedded in a homogeneous isotropic turbulent flow [3–5], jet flames [6–9]). Few studies treat relatively more complex geometries and realistic burners [10–13]. One main reason explains this situation. Combustion and turbulence behave very differently: most of the turbulence energy is resolved in LES, a way to check simulation quality [14], while combustion is mainly a sub-grid scale phenomenon, possibly leading to an ill-posed problem when looking for a linear parameter in a dynamic procedure [4].

Flame front wrinkling factors, quantifying flame/turbulence interactions in terms of ratio of total to resolved flame surfaces in the filter volume enter directly flame surface density (FSD) [15], thickened flame (TFLES) [16,17] and F-TACLES [18] models. They also may be used to model the sub-grid scale turbulence flame speed in level-set formalism [6,19]. Charlette et al. [4] proposed a global dynamic formulation where the spatially-uniform time-dependent exponent parameter of a fractal wrinkling factor expression is determined automatically. Wang et al. [5,7] have shown the ability of such a dynamic model to reproduce a statistically steady jet flame [20] and the transient ignition of a flame kernel [21] under several operating conditions. The TFLES model was used in the first case while the second retained the Boger et al. algebraic FSD model [15]. Knikker et al. [22,23] proposed a Dynamic Flame Surface Density (DFSD) model based on a fractal analysis [24,25] and on a similarity assumption [26]. This model was validated a priori from experimental data and, more recently, tested a posteriori by Ibrahim et al. [12] and Gubba et al. [13] to simulate the propagation of a turbulent premixed flame through obstacles in a laboratory scale combustion chamber.

Using the level-set formalism, Knudsen and Pitsch [6] performed simulations where the parameter of a model expression

* Corresponding author.
E-mail address: denis.veynante@ecp.fr (D. Veynante).

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for the sub-grid scale turbulent flame speed depends on both space coordinates and time. Schmitt et al. [8,10] adopted a similar strategy coupling a dynamic fractal wrinkling factor expression with the tabulated chemistry F-TACLES method. They simulated the Tecflam turbulent swirl burner [27,28] and, later, turbulent Bunsen flames [20] over three different operating conditions. Volpiani et al. [9] simulated the F3 jet flame studied by Chen et al. [20] and investigated the influence of physical and numerical characteristics of a flame wrinkling factor dynamic model for both, global (i.e. spatially-uniform time-dependent) and local (space and time dependent) model parameters. A similar local flame wrinkling factor dynamic formalism, combined with the Boger et al. model [15], gives very promising results to predict the development of a flame kernel in an internal combustion engine [29], even if an adapted ignition model remains to be developed.

Other authors applied the dynamic formalism to compute variances and scalar dissipation rates of a mixture fraction, that enter non-premixed combustion models [30–34]. These procedures can be denoted "indirect approaches", to differ from the previous one that involve directly reaction rate terms.

The goal of this paper is to apply the TFLES combustion model coupled with global and local dynamic procedures in simulations of a realistic burner configuration and to assess the influence of the dynamic model in the prediction of combustion instabilities. The chosen configuration is the PRECCINSTA swirl burner derived from a gas turbine designed by Turbomeca. This configuration has been the subject of many experimental [1,35] and numerical [36–41] studies. Experimental studies using the PRECCINSTA burner evidenced two combustion regimes [1]: a quiet flame at equivalence ratio $\phi = 0.83$ and a pulsating flame at $\phi = 0.70$. Numerical simulations commonly assume perfect mixing between fuel and air at the combustion chamber inlet because in the experiment methane is injected in the swirler, far upstream of the combustor. However, in the configuration where self-excited combustion oscillations are found, simulations assuming perfect mixing fail to predict the combustion instability [42].

The paper is organized as follows: basic concepts of the TFLES combustion model are first reviewed. The dynamic procedure is then briefly discussed. Experimental and numerical set-ups are presented. Numerical results are then compared to experiments and discussed for both stable and unstable cases. Conclusions are drawn.

2. Modeling

2.1. The thickened flame model (TFLES)

Flames are artificially thickened to be resolved on the numerical grid by multiplying diffusion and dividing reaction rates by a thickening factor $\mathcal{F}$ but conserving the laminar flame speed S_L [43,44]. An efficiency function is added to correct the reduction of flame surface induced by the thickening operation [16,17]. Charlette et al. [17] express this term as a sub-grid scale wrinkling factor, Ξ_Δ, that measures the ratio between the total and the resolved flame surface. Thus, the balance equations for filtered species mass fractions $\widetilde{Y}_k$ are written as:

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

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 [45,46] and $\dot{\omega}_k$ the reaction rate of species k, estimated from Arrhenius laws. Any quantity $\overline{Q}$ corresponds to the filtering of the Q-field, while $\widetilde{Q} = \overline{\rho Q}/\overline{\rho}$ denotes mass-weighted filtering. Similarly, the balance equation for the filtered total energy $\widetilde{E}$ is written:

$$\frac{\partial \overline{\rho}\widetilde{E}}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}\widetilde{E}) = -\nabla \cdot \left[\widetilde{\mathbf{u}}\overline{P} - \widetilde{\mathbf{u}}\,\overline{\boldsymbol{\tau}} + \Xi_\Delta \mathcal{F} \left(\overline{\mathbf{q}}_T - \sum_{k=1}^{N} \overline{\rho \mathbf{V}_k} \widetilde{Y}_k \widetilde{h}_{s,k} \right) \right] + \frac{\Xi_\Delta}{\mathcal{F}} \dot{\omega}_T(\widetilde{Q}) \tag{2}$$

where $\overline{P}$ is the filtered pressure, $\widetilde{h}_{s,k}$ the sensible enthalpy of species k, $\overline{\boldsymbol{\tau}}$ the viscous tensor, $\overline{\mathbf{q}}_T$ the thermal flux due to temperature gradients modeled using a Fourier law and $\dot{\omega}_T$ the heat release rate. Eqs. (1) and (2) propagate a flame front of thickness $\mathcal{F}\delta_L^0$ at the sub-grid scale turbulent velocity $S_T = \Xi_\Delta S_L$, where δ_L^0 is the laminar flame thickness.

2.2. Dynamic wrinkling model

Charlette et al. modeled the wrinkling factor Ξ_Δ by an algebraic expression derived assuming an equilibrium between turbulence motions and flame front wrinkling [17]:

$$\Xi_\Delta = \left(1 + \min\left[\max\left(\frac{\Delta}{\delta_L^0} - 1, 0 \right), \Gamma_\Delta \left(\frac{\Delta}{\delta_L^0}, \frac{u'_\Delta}{S_L}, Re_\Delta \right) \frac{u'_\Delta}{S_L} \right] \right)^\beta \tag{3}$$

where 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. Note that the (-1) contribution in Eq. (3) was introduced later [7] to recover Eq. (4) below in the limit of large turbulence intensities. In practice, Eq. (3) is often saturated and dominated by Δ/δ_L^0, reducing to [47]:

$$\Xi_\Delta = \left(\frac{\Delta}{\delta_L^0} \right)^\beta \tag{4}$$

corresponding to a fractal model with a flame surface of fractal dimension $D = \beta + 2$ and an inner cut-off scale sets to the laminar flame thickness δ_L^0 [24,48,49]. The exponent β is now determined dynamically equating flame surfaces when computed at filtered and test-filtered level (Germano-like identity) [5,8,47,50]:

$$\left\langle \widehat{\Xi_\Delta |\nabla \widetilde{c}|} \right\rangle = \left\langle \Xi_{\gamma\Delta} |\nabla \widehat{\widetilde{c}}| \right\rangle \tag{5}$$

where c is the progress variable, estimated here from temperature, and the hat symbol denotes a test-filtering operation. The effective filter size when combining two Gaussian filters of size Δ and $\widehat{\Delta}$, is $\gamma\Delta$, with

$$\gamma = \sqrt{1 + \left(\frac{\widehat{\Delta}}{\Delta} \right)^2} \tag{6}$$

Symbol $\langle \cdot \rangle$ denotes an averaging operator [4] that may be the overall computational volume (*global formulation*) or a small local volume (*local formulation*). For the latter case and following [47,50], the averaging operation is here replaced by a Gaussian filter Δ_{avg}, easier to implement on massively parallel solvers with unstructured meshes [39]. Combining Eqs (4) and (5) and assuming that β is constant over the averaging domain $\langle \cdot \rangle$ give:

$$\beta = \frac{\log \left(\left\langle \widehat{|\nabla \widetilde{c}|} \right\rangle / \left\langle |\nabla \widehat{\widetilde{c}}| \right\rangle \right)}{\log(\gamma)} \tag{7}$$

However, strictly speaking, a thickened flame is not a filtered flame following the standard LES definitions and an equivalent filter size Δ should be specified to enter relations (4) and (6). As the