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Analysis of dynamic models for large eddy simulations of turbulent premixed combustion

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ABSTRACT

Dynamic procedures to automatically determine flame wrinkling factors from known resolved fields in large eddy simulations of turbulent premixed combustion are investigated from a priori tests processing a DNS database of a turbulent swirled flame. These flame wrinkling factors measure the ratio of total to resolved flame surfaces in the filtering volume and enter directly or indirectly into various flamelet combustion models through the sub-grid scale turbulent flame speed. They are usually modeled by algebraic expressions derived assuming equilibrium between turbulence motions and flame dynamics, a situation generally not reached during early stages of flame developments. Dynamic models then appear as a promising alternative to flame wrinkling factor or flame surface density balance equations to handle out-of-equilibrium situations. Attention is paid to three key requirements: *(i)* the correct prediction of propagating laminar flame fronts; *(ii)* the replacement of the averaging volume introduced to determine resolved and test-filtered flame wrinkling factors by a Gaussian operator easier to implement on unstructured meshes and/or massively parallel machines; *(iii)* the use of a local model parameter, evolving both in space and time. The two first requirements suggest basing the procedure on flame surface conservation instead of on chemical reaction rates. The saturated form of the Charlette et al. efficiency function [1], $\Xi_\Delta = (\Delta/\delta_l)^\beta$, where Δ is the filter width and δ_l the flame thickness, is found to be very well suited to dynamic determination of the model parameter β, easy to implement and very robust in practice, as confirmed by preliminary a posteriori tests.

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1. Introduction

Large eddy simulations (LES) is now widely used to describe turbulent premixed combustion [2–4]. The largest turbulent motions are explicitly computed while only the effects of the smallest ones are modeled, reducing the contribution of the model compared to RANS (Reynolds Averaged Navier–Stokes equations). Moreover, this technique gives access to unsteady flame behaviors as encountered during transient ignition [5], combustion instabilities [6–9] or cycle-to-cycle variations in internal combustion engines [10–13]. The unresolved flame / turbulence interactions may be modeled in terms of sub-grid scale turbulent flame speed [3], flame surface density [11,14,15] or flame surface wrinkling factor [1,16–18]. Most of these models assume an equilibrium between turbulence motions and flame surface wrinkling, expressed through algebraic expressions which are not adapted to transient situations. For example, such an equilibrium is generally not reached during the early stages of the flame development: initially laminar flame elements are progressively wrinkled by turbulence motions as convected downstream (jet flames) or during the growing of a flame kernel (internal combustion engines) [11]. A solution to handle non-equilibrium situations is to solve an additional balance equation for the flame surface density [11,15] or the flame wrinkling factor [16].

Dynamic models, taking advantage of the known resolved flow field to automatically adjust model parameters during the simulation, appear as a very promising alternative. As sub-grid scale reaction rates are more or less directly related to resolved reaction rates, dynamic models are a priori able to handle situations where an equilibrium has not been reached yet between turbulence motions and flame movements. However, while this formalism is routinely used for unresolved transport since the pioneering work of Germano et al. [19], relatively few attempts have been made to develop combustion dynamic models [3,4]. First, dynamic modeling induces an extra computational cost that could be non negligible in expensive reacting flow simulations and/or on unstructured meshes due to the implementation of the test filtering procedure. Also, momentum transport and combustion behave differently: most of the turbulence energy lies in resolved scale motions, a way to check LES quality [20], while

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combustion is mainly a sub-grid scale phenomenon. Looking for a parameter modeling the sub-grid scale contribution by a linear expression may then lead to an ill-posed problem [21].

Dynamic approaches in turbulent combustion may be classified into two categories. "Indirect" procedures apply the dynamic formalism to the description of the turbulent mixing through variances and scalar dissipation rates of a mixture fraction, that enter non-premixed combustion models [3,22–26]. On the other hand, "direct" approaches directly proceed with reaction rates through scale similarity assumptions [27], turbulent flame speed [3,28] or flame wrinkling factors [21,29–35], but concern turbulent premixed flames.

Recently, Wang et al. [30,31] show the ability of a dynamic flame wrinkling factor model to reproduce a statistically steady jet flame [36] and the transient ignition of a flame kernel, respectively, under several operating conditions, looking for an unique parameter over the flow field, evolving only with time. The objective of this work is to go further in the analysis, the formulation and the practical implementation of flame wrinkling factor dynamic models. This wrinkling factor is a basic ingredient to describe interactions between flame fronts and turbulence motions in several turbulent combustion models such as Level-Set [3,28], Thickened Flame Model [1,17], algebraic flame surface density models [14] or the recently developed F-TACLES (Filtered Tabulated Chemistry for LES) approach [18] to incorporate complex chemistry features in LES. Our attention is focused on: *(i)* the recovery of the correct propagation of a laminar premixed flame, as practically observed during the early stages of flame developments; *(ii)* the use of a local model parameter, previous computations [30,31] being limited to a spatially uniform parameter evolving only with time; *(iii)* the practical implementation of dynamic models (optimised model formulation, test-filter size, averaging volume to avoid numerical inconsistencies, ...).

Our analysis is based on DNS data of the lean premixed swirled PRECCINSTA turbulent flame [37,38] briefly described in Section 2. Then, the theoretical derivation (Section 3) is supported by a priori tests (Section 4). A posteriori tests of the same configuration are presented in Section 5.

2. Direct numerical simulation (DNS) data

Both the a priori and a posteriori analysis are performed in the lean-premixed PRECCINSTA burner, which was investigated experimentally at DLR [39]. This configuration was specifically designed for the validation of Large-Eddy Simulation combustion models [8,40–44]. The Reynolds number at the injector exit is moderate around 40,000, and it operates with a lean mixture of air and methane which leads to a laminar flame thickness of 424 microns when evaluated from the maximal temperature gradient. The integral and Kolmogorov length scales were estimated with highly resolved LES around 7.0 mm and 29 microns, respectively. These scales lead to Damköhler and Karlovitz numbers around 7.5 and 7.2 respectively. This burner is therefore particularly well suited for the present study as the spectrum of time and space scales is large but remains accessible with current super-computers when using a tabulated chemistry approach.

The a priori study is conducted from a DNS simulation based on the Flamelet Prolongation of ILDM (FPI) closure for detailed chemistry [68]. This database was generated for the a priori analysis of the Presumed Conditional Moment (PCM) closure [38]. The calculation counts 2.6 billion cells, with a homogeneous mesh size of 85 micrometers in the flame region. The term DNS is used here as the laminar flame is resolved with around ten points inside its thermal thickness and this mesh size is sufficient to resolve the progress variable source term (about five mesh points inside the thickness evaluated from the maximum progress variable gradient) and the small turbulent scales with three Kolmogorov scales per mesh size in the fresh gases. In the burnt gases, turbulence is largely over-resolved due to the kinematic viscosity increase. The calculation cannot be considered as a DNS in the swirler as the maximum wall distance is around ten in wall units.

The DNS was generated with the finite-volume YALES2 code, which has been designed to handle very large meshes thanks to multi-level partitioning (www.coria-cfd.fr/index.php/YALES2). The code solves the low-Mach number Navier–Stokes equations with a projection method for variable density flows and fourth-order finite volume schemes. The run was performed on 16,384 cores of an IBM Blue Gene/P machine at IDRIS in France. Details on the DNS may be found in references [37,38]. Figure 1 displays an instantaneous temperature field as extracted in the medium plane of the DNS. A reduced part of the database, centered on location $x_0 \approx 1.4$, $y_0 \approx 0.32$, $z_0 \approx -2.0$ cm (see Fig. 1) and easier to manage on laptop computers, is also considered for some a priori tests. Moreover, turbulence and flame characteristics may be assumed to be homogeneous over the corresponding volume of $5.6 \times 6.3 \times 4.1\,\text{mm}^3$, a convenient property to investigate modeling.

3. Theory and modeling

3.1. Progress variable balance equation and generic formulation of the reaction rate

The description of the turbulent premixed combustion is based on a reaction progress variable c monotonically increasing from $c = 0$ in pure fresh gases to $c = 1$ in fully burnt products. The filtered progress variable balance equation reads:

$$\frac{\partial \overline{\rho}\widetilde{c}}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}\widetilde{c}) = \nabla \cdot \overline{\mathcal{J}} - \nabla \cdot [\overline{\rho}(\widetilde{\mathbf{u}c} - \widetilde{\mathbf{u}}\widetilde{c})] + \overline{\dot{\omega}(c)} \tag{1}$$

where t is the time, ρ the density, $\mathbf{u}$ the velocity vector, $\mathcal{J}$ the molecular diffusion flux and $\dot{\omega}(c)$ the progress variable reaction rate. Any quantity $\overline{Q}$ corresponds to the filtering of the Q-field, while $\widetilde{Q} = \overline{\rho Q}/\overline{\rho}$ denotes mass-weighted filtering. Only Gaussian filters will be considered in the following. The LHS terms in Eq. (1) are unsteady terms and convection by the resolved flow field, respectively, while RHS terms denote molecular diffusion, unresolved scalar transport and filtered reaction rate, respectively, and require closures.

Following Charlette et al. [21], the filtered reaction, $\overline{\dot{\omega}(c)}$, is written under the generic form:

$$\overline{\dot{\omega}(c)} = \Xi_\Delta \frac{W_\Delta(\widetilde{c})}{\sqrt{\Delta^2 + {\delta_l}^2}} \tag{2}$$

where $W_\Delta(\widetilde{c})/\sqrt{\Delta^2 + \delta_l^2}$ corresponds to the resolved reaction rate, estimated from filtered quantities such as the mass-weighted filtered progress variable $\widetilde{c}$ (note that c and $\widetilde{c}$ stand here for any quantity entering the reaction rate). Δ is the LES filter size. The wrinkling factor Ξ_Δ measures the ratio of total to resolved flame surfaces in the filtering volume. The original expression, $\overline{\dot{\omega}(c)} = \Xi_\Delta W_\Delta(\widetilde{c})/\Delta$ [21], is slightly modified here, introducing the laminar flame thickness δ_l to ensure a correct behavior and suitable comparisons with DNS when $\Delta \to 0$. Of course, the original expression is recovered when the filter size is far larger than the laminar flame thickness.

Expression (2) holds as long as flame / turbulence interactions are described in terms of flame surface wrinkling factor or sub-grid scale turbulent flame speed $S_T = \Xi_\Delta S_l$ where S_l is the laminar flame speed (flamelet assumption). Table 1 summarizes $\overline{\dot{\omega}(c)}$ and W_Δ expressions for several models: the Boger et al. [14,45] algebraic model, extending the Bray-Moss-Libby formalism [46] to LES, the level-set, or "G-equation", approach [3], the thickened flame model [17] where the thickening factor is here given in terms of flame thickness and filter size as $F = [(\Delta/\delta_l)^2 + 1]^{1/2}$ or the F-TACLES model where resolved reaction rates, as well as transport and diffusive terms in the filtered progress variable balance equation, are modeled from filtered one-dimensional laminar premixed flames [43,47].

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