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DNS and approximate deconvolution as a tool to analyse one-dimensional filtered flame sub-grid scale modelling

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ABSTRACT

A procedure using approximate deconvolution and explicit filtering is discussed to evaluate topology-based sub-grid scale (SGS) combustion models. A direct numerical simulation (DNS) database is first filtered, then a deconvolution operator constructed from the topology-based SGS model is applied, to compare the approximate three-dimensional fields against the exact ones. The DNS is obtained from an already well-resolved large eddy simulation (LES) of a bunsen flame, by refining the mesh up to full resolution of the reaction zones and the turbulent flow scales. The SGS model evaluation *via* approximate deconvolution is applied to a flamelet-like closure based on the tabulation of filtered one-dimensional flames. The various sources of errors are analysed in a statistical manner in terms of flame topology. Aside from the *a priori* analysis, results from LES are also reported with the one-dimensional flame deconvolution and compared against those resulting from an approximate three-dimensional deconvolution, confirming the need for accounting for the full 3D flame dynamics in SGS modelling. All the study is performed with tabulated detailed chemistry.

1. Introduction

Canonical flame problems, such as one-dimensional premixed flames, have been used very early to analyse turbulent combustion and develop numerical simulations [1–5]. Premixed flamelet modelling was applied successfully to a large variety of burners, within the Reynolds Average Navier Stokes (RANS) [2,6–9] and the Large Eddy Simulation (LES) [10–20] modelling frameworks. First introduced in the modelling to secure fundamental properties of premixed reaction zones, such as the flame speed, premixed flamelet modelling was then extended to chemistry tabulation of intermediate species and pollutants [21–24]. This requires the projection of the species profiles in a composition space defined from a progress variable monotonously evolving from fresh to burnt gases [25–27]. To account for the unresolved fluctuations, an averaging (RANS) or a space-filtering (LES) procedure needs to be applied to the flamelet responses prior to the simulations. The mean (or filtered) species concentrations are thereby related in a lookup table to the statistical moments of the progress variable, which are available on the mesh nodes. Other quantities used to calibrate the flamelet sub-grid scale model may also be involved, namely the equivalence ratio, the enthalpy for non-adiabatic cases, the rate of strain or the scalar dissipation rate of the progress variable. The flamelet may also be attached to a propagating scalar field (G-Equation) [28] or combined with a flame surface density approach [29].

One of the major strength of premixed flamelet based modelling lies in the fact that all the thermochemical quantities of the three-dimensional simulations will stay bounded within the physical values they take in the laminar flames. The first benefit is to help securing the stability and the convergence of the computations, the second is that the statistical properties of the scalars will also stay within these expected physical bounds, by construction.

Because of the filtering (or averaging) procedure, which must be combined with the canonical premixed flamelet to address three-dimensional turbulent flames of practical interest for which measurements exist, the capability of the one-dimensional flamelet in itself to represent the exact flow field may be difficult to assess directly. Henceforth, as for any modelling assumptions, it is mostly the comparison of global statistical quantities against their experimentally measured counterpart, which allows for concluding on the validity of the numerical tools.

Following the continuously increasing computing power, simulations have been reported in the literature for a large variety of resolution levels. It was analysed how simulations may, or may not, take advantage of the compensation of errors, whose source may be the numerical discretisation or the sub-grid scale modelling itself [30]. To progress in this direction, in the present work, LES and Direct Numerical Simulation (DNS) are combined with

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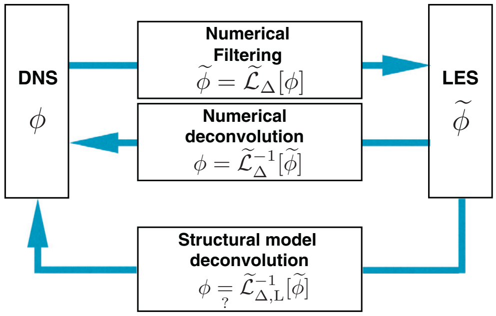

Fig. 1. Schematic of the filtering/deconvolution procedure. $\widetilde{\mathcal{L}}_\Delta^{-1}$: Inverse filtering deconvolution. $\widetilde{\mathcal{L}}_{\Delta,\mathrm{L}}^{-1}$: One-dimensional filtered flamelet deconvolution.

approximate filtering and deconvolution. The aim is to study, in an LES sub-grid scale modelling framework, the departure between the three-dimensional premixed turbulent reaction zones, and, the response of widely used closures based on one-dimensional and unstrained laminar flames. The ultimate objective is to determine up to which limit of flow resolution by the mesh, the one-dimensional flamelet assumption can survive. Indeed, in a weakly resolved flow simulation, such topology-based models are combined with a sufficiently high level of averaging/filtering, so that errors may be averaged and benefit from various compensation mechanisms, to provide in the end a modelling tool which appears as a very good compromise for coarse meshes. In other words, with the application of high-performance computing to the simulation of reacting flows, the role of the model is reduced on the one hand, because most of the flow fluctuations are resolved. But on the other hand, the absolute error of the model may be enhanced, because it cannot benefit from global averaging over a large amount of fluctuations, associated with error compensation. Therefore, it is interesting to measure the level of error induced by a closure when the assumed flame topology is directly applied to reconstruct the unresolved flow scales.

Approximate deconvolution and explicit filtering was discussed in the LES literature to tackle SGS transport by unresolved fluctuations [31–33] and also to simulate turbulent flames in the context of well resolved LES [34–37]. The deconvolution operator is based on a simple numerical treatment of the LES signal. The inversion of a discrete filter is derived in physical space from a Taylor expansion of a well defined filtering operation, leading to explicit or implicit inverse filters [38,39], which are directly applied to the three-dimensional scalar signals over the LES grid. The non-linear terms, as the chemical sources, are then computed from the deconvoluted signals, to be filtered back over the LES mesh to advance the solution in time. Obviously this approach dealing with signal reconstruction cannot be applied to LES with too coarse grids. In the case of bounded scalars and chemical sources, additional interpolations may be required within the sub-grid for sake of numerical stability, also an implicit filtering operation is usually preferred, because mathematically it returns the original DNS value in a back and forth filtering-deconvolution process.

The numerical deconvolution operator may also be replaced by a structural model based on physical hypotheses, which have been formulated to approximate the structure of the flame within the sub-grid. This allows for building from DNS, a tool to measure the various errors that will be brought by a given SGS flame closure within an LES context (Fig. 1). The DNS is filtered in space and the instantaneous fields reconstructed from the SGS physical model are then compared against their DNS counterparts. This may be done for various levels of filtering, combined with various conditional averaging, in order to better visualise the error introduced by the modelling.

In a first part, the grid is refined in a sub-domain of the LES of a premixed turbulent jet flame, up to full resolution of the signals, in order to reach DNS. The configuration is similar to the one experimentally studied by Chen et al. [40], but with an adiabatic pilot flame. The deconvolution applied to the filtered DNS signals should exactly reproduce the original fully resolved flames, as it is obviously the case with the filtering/approximate deconvolution based on a three-dimensional numerical treatment of the fields (Fig. 1). However, when introducing the one-dimensional filtered flame model into the deconvolution loop, errors are observed in the topology of the flame surface and the distributions of scalar fields. Specifically, these errors are found to be correlated with the properties of the local topology of the flame, which is parameterised for a range of filter sizes in terms of sub-grid scale flame wrinkling and curvature.

To further investigate these observations, and measure to which extent one-dimensional filtered flames may be used as a sub-grid scale closure, LES of the piloted jet flame is discussed in the configuration of the experiment [40]. Statistical results are obtained with a sub-grid scale closure based on a deconvolution operator assuming a one-dimensional flamelet structure within the sub-grid. They are compared against experiments and statistics previously collected in LES based on three-dimensional direct approximate deconvolution and explicit filtering [37]. Overall, the departure to measurements is found to be more pronounced with the one-dimensional flame deconvolution, confirming the DNS results.

Section 2 summarises the flame generated manifold context, in terms of the one-dimensional flame chemistry tabulation and the one-dimensional filtered flame tabulation. Section 3 reports on three-dimensional discrete filtering and deconvolution of scalar fields and a parallel is drawn with a well-established SGS mixing modelling. Two options for combining approximate deconvolution with flame tabulated chemistry are then addressed in Section 4. In the first option, the filtered progress variable field is deconvoluted with a three-dimensional discrete operator aside from the one-dimensional flame structure. In the second option, the inverse relation between the progress variable and its filtered value is tabulated from one-dimensional filtered flames and used as a deconvolution operation. The Section 5 is devoted to the parameters of the DNS embedded within the highly-resolved LES of the jet flame, and used to perform the *a priori* tests of approximate filtering and deconvolution. From this database, a statistical analysis of modelling errors is performed and conclusions are drawn for modelling based on one-dimensional filtered flames, in the context of well-resolved flow simulations. Finally, from additional LES of the jet flame, in Section 6, the statistical properties of the unsteady simulations involving deconvolution and approximate filtering, both based on discrete operators, or incorporating the flamelet hypothesis in the deconvolution step, are compared against measurements.

2. Flame generated manifold context

2.1. One-dimensional flame chemistry tabulation

In premixed flame tabulated chemistry approaches [21,41], one-dimensional flames are first computed with a detailed chemical kinetics, to collect the distribution of any thermochemical variable $\phi = \phi_L(\xi)$. A progress variable $c_L(\xi)$ is defined as a continuously growing function of ξ, the position through the flame [25–27]. Then, $\xi = \xi(c_L)$ is a unique function, providing the knowledge of ϕ versus c_L:

$$\phi = \phi_L(\xi(c_L)) = \phi_L^{\mathrm{Tab}}(c_L), \quad (1)$$