DYNAMIC MODELLING OF SUBGRID SCALAR DISSIPATION RATE IN PREMIXED AND PARTIALLY PREMIXED FLAMES WITH DIFFERENTIAL FILTER

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Abstract
Two test-filtering approaches for LES, based on algebraic and differential equations, are tested for flame configurations at different levels of turbulence. The analysis shows that the differential filter, unlike the algebraic one, is able to mimic also situations of weak turbulence, at the expense of a computational cost up to three times higher.

Introduction
Accurate and cost-effective modelling approaches are required to aid the design of new-generation gas turbines, able to meet the low-emissions targets set by the Paris agreement. Computational fluid dynamics is a powerful tool to predict the complex flow features within this design process. Among various techniques, LES represents a viable compromise between affordable computational cost and accurate prediction of the turbulent flow field. In a LES only large scales are resolved, with models to mimic the effect of the small, subgrid scale (SGS) motions. Since combustion is a small-scale phenomenon [1], the turbulence-combustion interaction must be modelled in a LES. An overview of different modelling approaches for LES of reacting flows can be found elsewhere [1].

The present work focuses on a flamelet-based combustion modelling approach with presumed probability density function (PDF). In this approach, a database of one-dimensional laminar premixed freely-propagating flames (flamelets) is used to describe all possible thermochemical states of the mixture. This database is accessed using a set of controlling variables, namely a Favre-filtered progress variable $\tilde{c}$, mixture fraction $\tilde{\xi}$, and their respective variances $\sigma^2_{c,sgs}$ and $\sigma^2_{\xi,sgs}$, whose Favre-filtered transport equations are directly solved in the LES (e.g. see [2, 3]). In this framework, the progress variable SGS scalar dissipation rate (SDR), $\tilde{\varepsilon}_c$, was shown to be a critical parameter for the correct estimation of $\sigma^2_{c,sgs}$. This term represents the unresolved part of the filtered SDR $\widetilde{N_c}$:

$$\bar{\rho}\widetilde{N_c} = \bar{\rho}\widetilde{D_c}(\nabla\tilde{c} \cdot \nabla\tilde{c}) + \bar{\rho}\widetilde{\varepsilon_c} \quad (1)$$

where $\bar{\rho}$ is the filtered density and $\widetilde{D_c}$ is the filtered diffusion coefficient of $\tilde{c}$. Models for $\widetilde{\varepsilon_c}$ are commonly proportional to the SGS variance and can be written in general form:

$$\widetilde{\varepsilon_c} = \frac{f_1 \sigma_{c,sgs}^2}{\beta_c} \quad (2)$$

where β_c is a modelling constant and f_1 is a function that can be more or less complex, and generally depends on turbulence and combustion parameters. Past works have shown that this function needs to account for the dissipation of both SGS turbulent and reactive processes and therefore simple approaches such as the linear-relaxation model are not suitable for this quantity [4]. In the present study the model originally proposed in [5] and then adapted for LES in [2, 4, 3] is used, and the reader is referred to these works for further details. The model constant β_c depends on flame curvature, diffusion and reaction processes, and is generally scale-dependent. Its choice is of crucial importance to obtain the correct estimation of SGS variance. Note that these considerations are generalizable also for the combustion constants in different modelling approach, although they may signify different processes. Thus, while the use of a static value of the combustion constant may lead to good results, it requires an accurate preliminary tuning. Furthermore, the value might need to change in space and time for cases where the aforementioned processes or the numerical mesh (thus the LES filter) is not homogeneously distributed, and for such case a single constant value might not be suitable.

Relatively recently, scale similarity assumptions for modelling parameters such as flame wrinkling and flame surface density have been proposed and investigated, e.g. see [6, 7, 8, 9]. Dynamic models based on the scalar dissipation rate have been also investigated [10, 2]. Although these models were observed to work on different regimes, the assumption of scale similarity is arguable for reacting quantities, and it is unclear whether the application of dynamic modelling leads to correct estimation of the modelling constant. An example was provided in [11], where it was discussed that on unstructured meshes the classical test-filter approaches based on Gaussian shapes lead to excessive noise and incorrect results due to the pseudo-Fourier condition [12]. Nevertheless, to the best of the authors' knowledge, a thorough investigation of the influence of the test filter in dynamic modelling for combustion LES still does not exist. In the present work we aim to fill this knowledge gap by investigating different techniques for test filtering, and testing the outcomes on two different configurations at different level of turbulence, in or- der evaluate the performance for different turbulent kinetic energy spectra. In particular, classical test-filtering approaches are compared to the so-called differential filters, where the general test filtered quantity $\hat{\bar{\phi}}$ is obtained through the resolution of a differential equation rather than the direct application of a Gaussian filter. This class of filters has been commonly used for non-reacting flows (e.g. see [13]), but not for reacting cases. In this work we discuss advantages and limitations of these from both modelling and computational cost sides. The analysis suggests that algebraic formulation only are acceptable at relatively high turbulence levels, while differential formulation provides good estimations for a much wider range of conditions and mesh type at the cost of a relatively marginal increase of computational effort.

Test cases and numerical details

For the analysis in the present work, two test cases are selected. The first, Case A, is the lean premixed, bluff-body stabilized flame studied in [14]. In this set-up, a low bulk velocity stream of (5 m/s) of methane/air mixture with at equivalence ratio 0.75 and inlet temperature of 300K is issued into a cylindrical duct with confinement ratio of $R_{out}/R_{in} = 2$ (see Figure 1a). This configuration leads to moderate levels of turbulence in the bluff body wake, where a recirculation zone is formed, which is ad hoc to compare the ability of the dynamic models for relatively narrow energy spectrum. The second case (Figure 1b), Case B, is the lifted partially premixed case in hot vitiated coflow developed by Dibble et al. [15]. The set up consists of a central nozzle issuing a fuel mixture composed of 25% H_2 and 75% N_2 in volume. The bulk velocity of the fuel stream is 107 m/s. This second case is therefore characterized by higher Re and a relatively wide turbulent kinetic energy.

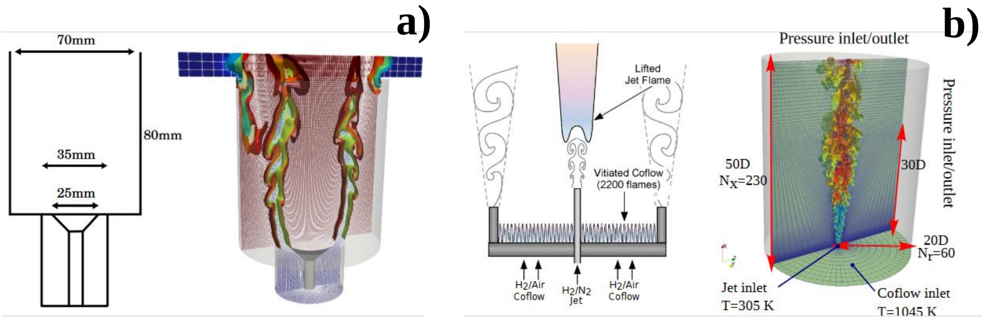

Figure 1. Sketch and numerical domain of the two test cases.

The hot coflow (1045 K) is composed of the products (H_2O, O_2 and N_2) of lean H_2/air flame at an equivalence ratio of $\phi = 0.25$. The two cases are simulated using an in house solver developed in OpenFOAM, which uses a low-Mach approximation and the PISO loop to solve the reacting Navier-Stokes equations along with the four transport equation for the controlling variables discussed in Sec. 1. An implicit Euler scheme is used for time marching along with a time step ensuring that the CFL number is everywhere below 0.3. Second order schemes are used for the spatial gradients, with Gamma limiters in the region of the flame where strong gradients are present. The mesh accounts to 2.5 and 0.9 million cells respectively for cases A and B, and are refined within the flame region to have a ratio between filter size and laminar flame thickness of about 1. Note that these meshes are structured, in order to avoid including additional uncertainty that one would have by the introduction of unstructured meshes, as discussed in [11]. Unstructured meshes will be explored in a future study.

Test cases and numerical details

Case A (bluff body), which is a weakly turbulent case, is analysed first. By looking at Fig. 2b, when the algebraic filter is used the dynamic procedure is not able to describe the local variations of the combustion model constant β_c across the flame region. The distribution of β_c assumes a bimodal distribution between the imposed boundary values, and $\beta_c \to 0$ in most of the domain (note that β_c in the numerical algorithm is truncated to $\varepsilon > 0$ to avoid a division by zero). This results in erroneous high values of the sub-grid SDR, and consequent low values of subgrid variance, which in turn implies the flame behaves as a laminar flame. This is not the case for this configuration, as could be observed from the OH-LIF images reported in [14]. Previous studies [16] highlighted the importance of the flame turbulence interaction, describing how the flame assumes a laminar-like behaviour close to the base of the bluff body and contributes to turbulence generation further downstream in the shear layer. From the comparison with the calculated non-reacting flow field, the flame appears to damp the weak turbulence generated in the shear layer around the bluff body, as a result of thermal expansion. The flame shape and regime can be qualitatively appreciated from the temperature fields in Fig. 2. On the other hand, the use of the differential filter results in a better calculation of β_c which now assumes a range of different local values across the flame front, and consequently higher values of $\sigma^2_{c,sgs}$ are obtained in the flame region. Note that also in this case the presence of the flame dumps the turbulence at the base of the bluff body, when compared to the non-reacting case (not shown). However, the formation of instabilities sustaining the turbulent structures in the shear layer can be observed further downstream. Test case B (jet flame in hot coflow) is analysed next. In this case the use of an algebraic Gaussian test-filter does not lead to a total failure of the numerical algorithm as for Case A. As can be seen from Fig. 2, the β_c field appears very similar to that predicted by The reason may be traced back to the higher level of turbulence associated with the high bulk velocity of the fuel jet. Overall, the local values of $\sigma^2_{c,sgs}$ are about 40% higher than the maximum values calculated in case A. This result suggests that the dynamic evaluation of β_c is less sensitive on the choice of the test filter at high turbulence. However, the different stabilization mechanism and combustion mode (purely premixed/partially premixed) might also affect the choice of test filter, and this will be investigated in a future study. Next, a scalability test on the 2.5 million cells mesh of case A is carried out to assess the additional computational cost of solving for the differential test filter. The results, reported in Fig. 3, show a 125%-370% computational time increase in seconds per iteration. One can thus conclude that for cases at high level of turbulence, differential filters might not be worth, although one has to be careful of quasi-laminar regions near the anchoring point [16]. Differential filters, however, allow to deal with these quasi-laminar situations and thus are more versatile. Note also that the present analysis was based on qualitative considerations. Quantitative considerations will be presented in a future study.

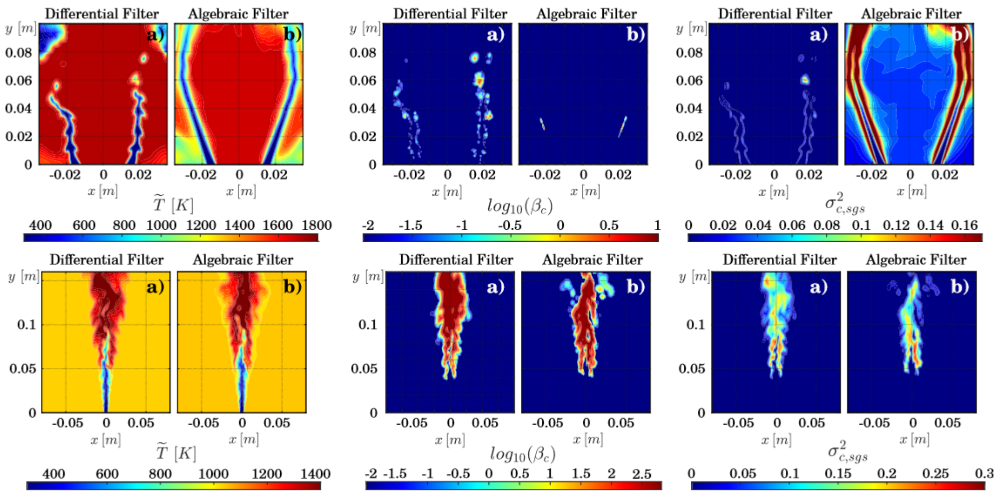

Figure 2. Comparison between instantaneous fields of temperature (left), combustion model constant (centre) and SGS variance of progress variable (right), as predicted using the algebraic and differential filters. Case A is shown on top, Case B on the bottom.

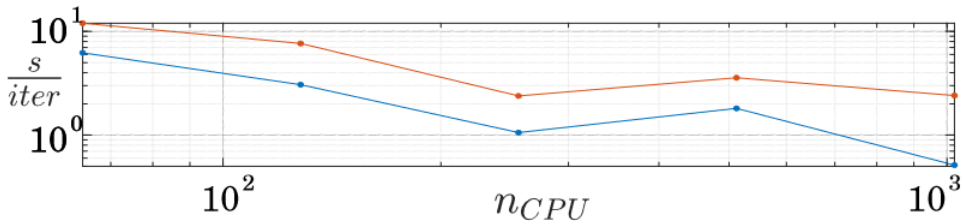

Figure 3. Scalability test: β_c computed via differential (red line) and algebraic (blue line) test filter.

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