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Analysis of a filtered flamelet approach for coarse DNS of premixed turbulent combustion

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HIGHLIGHTS

- Premixed combustion modeling regimes based on subgrid turbulence level.
- Flame reconstruction from 1-D laminar flame solution filtered at mesh width.
- A *priori* and a *posteriori* analysis of filtered flamelet approach for coarse DNS.

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ABSTRACT

Nowadays numerical simulations of premixed turbulent combustion can be performed at high spatial resolutions due to the continuously increasing computational power. At a resolution of the order of the laminar flame thickness there is negligible turbulence in the subgrid level and a proper reconstruction of the filtered flame is adequate for accurate predictions. In this scenario, which can be termed as a coarse scale Direct Numerical Simulation (DNS), reconstruction of the filtered flame using a spatially filtered flamelet (1-D laminar flame) is analysed. First, DNS of a turbulent premixed slot burner is computed to generate a reference database. This database is filtered at different length scales of the order of laminar flame thickness for an *a priori* assessment of turbulent flame reconstruction using a filtered flamelet. The filtered DNS source term, molecular diffusion and subgrid convection of the reaction progress variable is compared with a flamelet convoluted with top-hat profiles of the same order. The source term and molecular diffusion are approximated well from the filtered flamelet while the unresolved convection shows deviation. Finally, the reconstruction of the turbulent flame is tested *a posteriori* on the same filter widths (mesh size) and the results are compared. It is found that a flamelet filtered spatially at the order of the computational mesh and tabulated using a single controlling variable i.e. the reaction progress variable is suitable for a coarse scale DNS of premixed turbulent combustion.

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1. Introduction

Today a significant part of our energy needs is generated with devices burning hydrocarbon-air mixtures. Limited fuel resources as well as environmental concerns call for design of efficient combustion systems. In order to do so, numerical prediction of combustion has become an indispensable tool. Technical combustion devices rely on turbulence to enhance the power generation and their operation mostly takes place in the thin reaction zones (TRZ) regime [1]. Besides turbulence modeling, reduction of the combustion chemistry is a vital step, and along with the Reynolds number it determines the computational cost.

Reduction of chemistry by using tabulated chemistry methods like Flamelet Generated Manifold (FGM) [2] or Flamelet Prolongation of Intrinsic Low Dimension Manifold (FPI) [3] enables prediction of intermediate species as well as pollutants [4]. This is achieved at much lower cost than using detailed mechanisms by decoupling chemistry from the flow and relaxing the resolution required for resolving the chemistry [5,6]. A common approach is to treat the reacting flow with Computational Fluid Dynamics (CFD), to solve the Navier–Stokes equations supplemented by an equation for a progress variable (c). A (reaction) progress variable is a scalar that tracks the progress of the chemistry and is bound between the unburnt (0) to a completely burnt (1) state. Recently, a Hybrid Transported-Tabulated Chemistry (HTTC) approach [7] is introduced in which all the species which are non zero in fresh and burnt gases are transported with the flow and an optimized progress variable is defined from them. This ensures proper prediction

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of intermediates species which are expressed based on their self similar properties. In order to model adiabatic premixed combustion, a single controlling variable i.e. the progress variable is adequate if there is no significant differential diffusion [2]. A manifold constructed using FGM, in which the source term of the progress variable is a function of the progress variable, is an integral part of the system.

Let us consider what happens when performing a numerical simulation. On a computer we have to consider a discretized system and thus a certain continuous neighborhood should be contracted to a point. This discretization in space, gives rise to a filtered description of the system. To be consistent, we also have to filter the manifold (in physical space). Now, if the size of the filter (Δ), which is implicitly applied to the system by the spatial discretization, tends to very small values, the system converges to DNS. For DNS of reacting flow, the filter size has to be small enough to resolve the reaction layer because in the TRZ regime of premixed turbulent combustion, the thickness of the reaction layer is smaller than the smallest fluid dynamic flow structures, defined by the Kolmogorov scale [1]. The latter scales can penetrate the preheat zone perturbing the flame structure but are too large to penetrate the reaction zone. Moreover, flow structures of the order of the Kolmogorov scale are only present in a temporal and spatial intermittent distribution (so not omnipresent). Therefore the strategy of using FGM for doing DNS of reacting flows in the TRZ regime is a good approximation as illustrated in e.g. [8].

As the mesh is coarsened and hence the filter size is increased, the flow will be gradually under-resolved starting with the reaction layer first. In particular, if the manifold would not be filtered, the source term would be misrepresented because there is insufficient resolution of the source term in physical space. If the filter size is of the order of the laminar flame thickness, there are negligible subgrid turbulent structures and the subgrid scale (SGS) variance then corresponds to the spatial resolution of the gradients produced by the reaction zone [9]. It is our assumption that in this scenario the subgrid scales can be determined from filtered flamelets. This assumption was verified in simulations of a turbulent Bunsen flame on a coarse grid with a mesh spacing of the order of the laminar flame thickness (δ_L) by Vreman et al. [10]. Here the term subgrid is used loosely to refer to phenomena that are unresolved, e.g., the reaction layer and does not necessarily mean that there are any turbulent structures at subgrid or subfilter level. Thus, by properly and consistently filtering the manifold we may be able to use relatively coarse grids to reduce the computational efforts.

With increasing filter size, filtered products of quantities start to deviate from products of these filtered quantities. Since only the filtered quantities are available, there is an additional closure problem that grows with filter size. This problem occurs mainly in two components of the transport equation of the progress variable: in the convective and in the diffusive terms. But here again, since we know the laminar flame structure we also know the error associated and can correct for it. Fiorina et al. [11] considered this issue and demonstrated that by proper modeling it is possible to recover the laminar burning velocity for a 1-D laminar flame on a coarse computational grid.

If we go to larger filter sizes, i.e., $\Delta > \delta_L$ and of order Taylor microscale (λ), then we can find turbulent subgrid events and gradually enter the region of under-resolved hydrodynamic turbulence. In this case a subgrid model is required for the momentum equation and the flamelets become corrugated within the subgrid scales. Now, the information of the laminar flamelets becomes too limited and turbulent information should be taken into account. Modeling this is possible through a probability density function (PDF) of the occurrence of subgrid values of the progress variable source term. In principle this PDF would be a function of the moments of the local turbulence, typically mean and variance [12]. Often a presumed distribution like the β-function is used because of its ability to describe a multiple set of behaviors. This includes Gaussian like behavior but also, uni-modal, bi-modal and constant behavior. All these modes rely on the support of only two quantities, the mean and the variance.

It is the observation of the authors that there is a difference between coarse scale (or filtered) DNS and LES. Most literature on turbulent (premixed) combustion is not sensitive to this difference. The first regime can be considered as a coarse scale DNS (or Filtered Numerical Simulations) where stochastic events are almost negligible and modeling is limited to deterministic events which can be recovered from a filtered flame structure. The second regime can be considered as typical LES of reacting flows where the flame is completely subgrid and the stochastic events can exist in subgrid. Therefore, we divide the turbulent combustion modeling problem into two regimes:

- flame information that is not taken into account but can be reconstructed;
- turbulent flow information that is generally unknown and needs a statistical modeling approach.

It is interesting to investigate combustion modeling using laminar flame information, starting from the first regime (coarse DNS) and as the resolution is coarsened up finally to the second regime (LES). Next, some available literature on the use of filtered laminar flame structure is discussed.

Filtered laminar flames have been investigated for modeling turbulent combustion by Boger et al. [13], Domingo et al. [14], Duwig [15], Vreman et al. [10], Fiorina et al. [11] and Moureau et al. [16]. Based on the filter size applied over the flame, these studies can be classified into two groups:

- flame filter size larger than computational mesh size [13–15,11];
- flame filter size of the order of the computational mesh size [10,16].

Some studies in the first group ([13,14,11]) use very large filter widths compared to the mesh size so that the filtered flame structure is resolved numerically by enough grid points in order to recover the correct laminar burning velocity like the Thickened Flame Model (TFM) [17]. However, in context of LES, the filtering operation is also applied to the velocity fields, unlike the thickening operation [15]. Further, the interaction of the filtered flame with subgrid turbulent structures is recovered through the use of a flame wrinkling factor or efficiency function. For example, a recent model F-TACLES [11] first attempts to recover the laminar flame speed (s_L^0) accurately and finally the turbulent burning velocity (s_T) is recovered by using a flame wrinkling factor. In F-TACLES the adequate resolution of the filtered laminar flame structure (i.e. over 5 grid points), is achieved by using very large filter widths. However, application of large filter width (e.g. 20 times δ_L [11]) changes the flame turbulence interaction from transport dominated to chemistry dominated regime. In addition, the flame wrinkling factor/efficiency function rather empirically modifies the source term and the molecular diffusion [1]. Duwig [15] performed successful LES of a dump combustor using a filter only 2 times the mesh/cell size to filter the flamelet and a small flame wrinkling factor.

In the second group of studies, the filter applied over the flamelet is of the order of the computational mesh size and the focus is on directly recovering the turbulent burning velocity. For example, Vreman et al. [10] used a flamelet spatially filtered with top-hat filter, of width equal to the computational mesh. The mesh size was of order of the laminar flame thickness, and resulted in good predictions for planar Bunsen flames in the TRZ regime. Moureau

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