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Investigation of lengthscales, scalar dissipation, and flame orientation in a piloted diffusion flame by LES

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Abstract

This work investigates the structure of a diffusion flame in terms of lengthscales, scalar dissipation, and flame orientation by using large eddy simulation. This has been performed for a turbulent, non-premixed, piloted methane/air jet flame (Flame D) at a Reynolds-number of 22,400. A steady flamelet model, which was represented by artificial neural networks, yields species mass fractions, density, and viscosity as a function of the mixture fraction. This will be shown to suffice to simulate such flames. To allow to examine scalar dissipation, a grid of 1.97×10^6 nodes was applied that resolves more than 75% of the turbulent kinetic energy. The accuracy of the results is assessed by varying the grid-resolution and by comparison to experimental data by Barlow, Frank, Karpetis, Schneider (Sandia, Darmstadt), and others. The numerical procedure solves the filtered, incompressible transport equations for mass, momentum, and mixture fraction. For subgrid closure, an eddy viscosity/diffusivity approach is applied, relying on the dynamic Germano model. Artificial turbulent inflow velocities were generated to feature proper one- and two-point statistics. The results obtained for both the one- and two-point statistics were found in good agreement to the experimental data. The PDF of the flame orientation shows the tilting of the flame fronts towards the centerline. Finally, the steady flamelet approach was found to be sufficient for this type of flame unless slowly reacting species are of interest.

Keywords: Large eddy simulation; Flamelets; Non-premixed; Artificial neural networks; Lengthscales

1. Introduction

Over the last 30 years, large eddy simulation (LES) has been developed into a powerful method to simulate turbulent flows. Compared to the competing approaches, LES has the inherent advantage that accuracy scales with computer-power: with growing effort, the LES solution converges into the solution of the accurate Navier–Stokes equations. Once an expensive tool for research only, the exponential growth in computer-power makes LES affordable for many applications. In turbulent combustion, this was shown impressively, for example in [1–4].

Large eddy simulation allows a time resolved description of flow, mixing, and flame structure. This enables classical combustion models to show their full potential. Hence, these known models should be "re-assessed" for LES application. This work uses the steady flamelet model and shows how capable this model is when used with LES. To rate the model, it must be tested on a

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well-examined benchmark flame. This work relies on the piloted jet flame "D," which is described by elaborate experimental data: Velocity fields by Schneider et al. (Darmstadt [5]), scalar-fields by Barlow and Frank (Sandia [6]), and even the structure of the flame by Karpetis and Barlow (Sandia [7]).

In addition, there were many numerical simulations of Flame D, often contributing to the workshop on turbulent non-premixed flames (TNF) [11]. To the authors' knowledge, Flame D was already simulated by the groups around Bilger, Chen, Echekki, Fuchs, Gass, Gore, Janicka, Jones, Lindstedt, Peters, Pitsch, Pope, and Roekarts (e.g. [8–10]). They tested many different combinations of models for flow, mixing, and chemistry. The turbulent flow was modeled by RANS, PDF-methods, one-dimensional turbulence, as well as LES. The mixing was described by different RANS-models, via PDF-methods, and also with LES. Finally, the chemical state was determined by full or reduced reaction mechanisms, by intrinsic low-dimensional manifolds, by conditioned moment closure (CMC), steady or unsteady flamelets or with an equilibrium assumption. Flame D may well be the best-investigated turbulent flame, which turns it into the ideal benchmark for modeling approaches.

Despite this, not many successful large-eddy-simulations of this flame are known to the author. In 1998, di Mare and Jones [11] presented a first 3D-LES of this flame, applying a simple flamelet model on a grid of 1.3×10^6 nodes. Steiner and Bushe [12] applied a simplified CMC model (Conditional Sourceterm Estimation) to an LES with 0.8×10^6 nodes in 1999. One year later, Steiner and Pitsch [13] produced very convincing results, using the computationally expensive unsteady flamelet-model and a grid of 1.0×10^6 nodes. Their excellent data that were improved further in 2002 [4] have often been quoted to underline the high potential of combustion LES.

Since 2002, new experimental data by Karpetis and Barlow [7] are available, suited for LES validation. These Line-Raman measurements, with simultaneous flame visualization by planar laser induced fluorescence (PLIF) of OH, provide information on scalar lengthscales, scalar rates of dissipation, and flame orientation.

The present work attempts to predict these newly available quantities, that require a very accurate description of flow and mixing. This is achieved with a fine cylindrical mesh of 1.97×10^6 nodes. The extension of the CFD cells towards the nozzle is of the same order as the probe-volume in laser diagnostics. A steady flamelet model, represented by artificial neural networks (ANN), is used together with LES. This approach will be shown to suffice for a good prediction of this flame.

2. Governing equations, modeling, and numerical procedure

Transport of mass, momentum, and mixture fraction are described by solving the favre filtered transport equations for momentum, density, and mixture fraction [14,15]. The subgrid scale stresses were determined by the Germano model [16], which leads to the eddy viscosity ν_t. Together with the turbulent Schmidt-number ($\sigma_t \approx 0.4$ [13]), this yields the turbulent diffusivity $D_t = \nu_t/\sigma_t$, which is needed to model the subgrid scalar fluxes and the filtered scalar dissipation rate $\widetilde{\chi} = 2(\widetilde{D} + D_t)(\partial\widetilde{f}/\partial x_i)^2$ [17–19]. Here, $\widetilde{D}$ is the filtered molecular diffusivity.

The mixture fraction formulation [20], together with a steady flamelet model [17], is used to project the mixture fraction field to density, viscosity, temperature, and species mass fractions. The subgrid distribution of the mixture fraction is described by a presumed-shape β-PDF. While that of the scalar dissipation rate is considered by a Dirac peak at the (modeled) filtered scalar dissipation rate. The chemical state is therefore a function of the filtered mixture fraction $\widetilde{f}$, the modeled subgrid variance $\widetilde{f''^2}$ [14], and the filtered scalar dissipation rate $\widetilde{\chi}$. Flamelet solutions were kindly provided by Wachter (Darmstadt University), using the GRI mechanism 3.0 [21].

Using an approach by Flemming et al. [22], artificial neural networks (ANNs) are used for the storage and interpolation of the flamelet libraries. The ANNs are trained with the steady flamelet solutions, integrated with the presumed β-PDF. Multi-layer perceptrons, consisting of two hidden layers of non-linear neurons and one linear output layer with a single neuron, as shown in Fig. 1 are deployed. The networks are adopted to project the input-vector $(\widetilde{f}, \widetilde{f''^2}, \widetilde{\chi})$ to the filtered output quantities (e.g., density, viscosity, and species mass fractions). For each quantity,

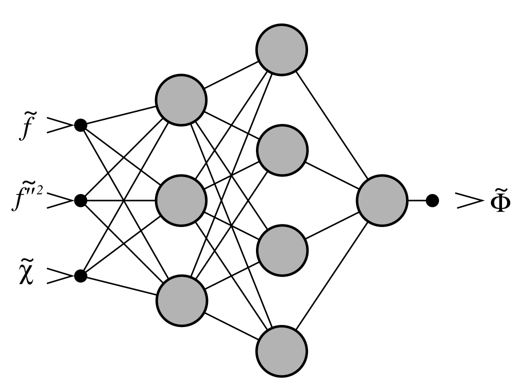

Fig. 1. Sketch of a multi-layer perceptron that represents the steady flamelet library. For each component of the vector of the chemical state, one artificial neural network is applied.