Large-eddy simulation of a turbulent piloted methane/air diffusion flame (Sandia flame D)

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1. Motivation and objectives

While numerical simulations of turbulent flows applying Reynolds averaging techniques solve equations for ensemble or time averaged mean quantities, Large-Eddy Simulations (LES) have the capability of resolving the major part of the turbulent kinetic energy of turbulent flows. Hence, only the influence of the small turbulent scales on the resolved field has to be modelled. Since, in addition, the small turbulent scales fulfill the common modelling assumption of isotropy much better than the large scales a very high accuracy in predictions of the turbulent flow field can be achieved by using LES. This is particularly interesting for simulations of chemically reacting flows, where an accurate description of mixing is essential and very complex phenomena like turbulent transition and instabilities might be of great importance.

The success of LES in predictions of turbulent flows is due to the fact that the kinetic energy content of the turbulent motion decreases with increasing wave number. Thereby, the major part of the Reynolds stresses is resolved. In the modeling of the unresolved part it is still most important to represent the larger scales of the unresolved part by a sub-grid scale model. However, since chemical reactions in non-premixed combustion occur only by molecular mixing of fuel and oxidizer, which in practical applications occurs only on the smallest scales, the combustion process occurs essentially at the sub-filter level, and has to be modeled entirely. This explains, why sub-grid modelling techniques, which have successfully been used in predictions of sub-grid scale stresses and variances might not necessarily be applicable in the modelling of the chemical source terms.

In recent years many studies have been devoted to a priori testing of the applicability of combustion models in LES (Cook *et al.* 1994, Cook & Riley 1997, Colucci *et al.* 1998, Cook *et al.* 1998, De Bruyn Kops *et al.* 1998, DesJardin & Frankel 1998, Bushe & Steiner 1999). Most of the proposed models have previously been used, or could very similarly be applied, in RANS calculations. Essentially, the proposed models can be divided into four categories: The direct method, the Linear-Eddy Model, the transported probability density function (pdf) method, and the conserved scalar method. Here, only the direct method and the conserved scalar method will be discussed.

Similarly as in RANS combustion models the direct modelling of the spatially filtered chemical source terms is a very challenging problem. Different direct closure models have been proposed by DesJardin & Frankel 1998. They first show that modelling the reaction term by only using the resolved scales gives very poor agreement compared to DNS results. This has also be shown in many other studies, for instance Colucci *et al.* 1998. In addition they propose two different direct

closure models based on the scale similarity assumption, which considerably improve the predictions, but are still not in good agreement with DNS data. The reason for this is obvious. The scale similarity assumption actually implies that the smallest resolved scales are statistically similar to the largest unresolved scales. This assumption seems to be very reasonable, but even though, it does not assist in the modeling of the chemical source term. As mentioned earlier, in turbulent non-premixed combustion, chemical reactions occur on the dissipative rather than the larger unresolved scales. This problem is inherent for all models, which estimate the reaction rates by only using the resolved scales and it explains why the combustion models applied in LES do not differ significantly from RANS combustion models.

The concept of sub-grid scale pdfs, introduced by Pope 1985, has also been used in the application of conserved scalar methods, which assume that the chemical state and thereby the species mass fractions can be related to a conserved scalar, for non-premixed combustion typically the mixture fraction. Then, by presuming the sub-grid scale pdf of the mixture fraction $\widetilde{P}(Z)$, the filtered species mass fractions $\widetilde{Y}_i$ in each computational cell can be evaluated by

$$\widetilde{Y}_i = \int_{Z=0}^{1} Y_i(Z)\widetilde{P}(Z)dZ, \tag{1}$$

provided the functional dependence $Y_i(Z)$ is known. Here and in the following the tilde denotes density weighted spatial filtering.

$\widetilde{P}(Z)$ is commonly assumed to follow a β-function distribution, parameterized by the first two moments of the mixture fraction. The filtered mixture fraction is determined by the solution of a transport equation, its sub-grid scale variance is typically given by a sub-grid scale model. The validity of the β-function representation of the pdf of the mixture fraction has been investigated by several authors using DNS data of non-premixed reacting flows for constant and variable density (Madnia & Givi 1993, Cook *et al.* 1994, Cook & Riley 1997, Jimenez *et al.* 1997, Cook *et al.* 1998, DesJardin & Frankel 1998). The two main conclusions are that the β-function pdf provides an excellent estimate for the sub-grid scale mixture fraction distribution and that this estimate is even much better for LES than for RANS models. This is shown to be particularly true, if the mixture fraction variance is taken from the DNS data, suggesting that the β-function as a model for the statistical distribution of the mixture fraction performs much better than the commonly used subgrid scale models perform for the mixture fraction variance.

The mixture fraction variance can be determined by standard sub-grid scale modelling methods like the scale similarity model as proposed by Cook *et al.* 1994, or by using a small scale equilibrium assumption and determining the remaining coefficient by the Dynamic Procedure following Pierce & Moin 1998. However, DesJardin & Frankel 1998, for instance, have shown that their modelling results do not differ if they use a δ-function instead of the β-function as sub-grid mixture fraction pdf in a conserved scalar approach. This conclusion depends certainly on the spatial resolution of the calculation and the turbulence intensity.