Application of flamelet generated manifolds to DNS of premixed turbulent spherical flames

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Keywords: DNS, flamelet generated manifolds, turbulent combustion, spherical flames, flame stretch

Flame stretch is recognised to have a determining effect on the burning velocity in premixed flames. The laminar burning velocity is an important parameter for modelling turbulent combustion. In the latter case, stretch rates vary significantly in space and time. An expression for the stretch rate is derived directly from its mass-based definition by de Goey and ten Thije Boonkkamp [2] and it is shown to consist of two terms. One term is due to the propagation of the flame itself and the other one is caused by the variation of the flame thickness. Detailed studies of the effect of flame stretch can also be performed both experimentally and numerically. In experiments, combustion tunnels and combustion vessels are used. In computer simulations, detailed chemical kinetics models can be applied nowadays to obtain accurate predictions. Recently calculations were carried out using a flamelet approach with a skeletal reaction mechanism and the theoretical corrections by Groot and de Goey [3]. The simulations were carried out with a one-dimensional code which is based on the isobaric approximation. Both spherical and cylindrical cases were studied for expanding, imploding and steady flames. It was shown that the model displays a good agreement with experiments, e.g. for the spherically expanding flames of Gu et al. [4] as in figure 1.

In order to test the ideas in turbulent combustion, direct numerical simulations (DNS) can be carried out. The term "direct" usually reflects the ability of such a method to resolve all the aerodynamic turbulent scales. For a properly chosen turbulence in combination with combustion also the chemical scales can be resolved. An example is the non-premixed reactive turbulent mixing layer as simulated using one-step chemistry by Bastiaans and de Lange [1]. This code with higher order discretisations is taken as a starting point for our turbulent combustion research. However, the use of detailed chemistry kinetics models in a DNS is quite beyond the capacity of present computing power. Application of chemical reduction techniques is an option to obtain meaningful DNS solutions, in which the effects of chemistry are taken into account in an accurate way.

A promising chemical reduction method as developed by van Oijen and de Goey [5] is the flamelet generated manifolds (FGM) technique. In this method the ideas of the manifold and the flamelet approach are combined: a manifold is constructed using one-dimensional flamelets. In [5], the effect of flame stretch on the accuracy of the FGM method is investigated. In order to isolate the effect of flame stretch, premixed methane/air counterflow flames are simulated. In the case of unit Lewis numbers a one-dimensional manifold is sufficient to model the main effects of flame stretch. A manifold with two progress variables reproduces the results computed using detailed kinetics almost exactly. When non-unit Lewis numbers are used, the enthalpy and element composition of the burnt mixture change, which may influence the mass burning rate significantly. If these changes are included in the manifold using one additional controlling variable, the results agree well with detailed computations.

The FGM method is applied in the DNS to study turbulent spherically expanding pre-

mixed flames. For a first validation the FGM technique was implemented in a one-dimensional version of the DNS. The results are shown in figure 2. It can be observed that the DNS gives a fast convergence with the number of grid points. In the converged result the DNS shows a slightly different laminar burning speed due to the fact that it is fully compressible in contrast to the reference method which adopts the isobaric assumption. Both computations are performed with second order one-step kinetics and unity Lewis numbers, tuned to the flame speed of calculations with GRI-mech 3.0. When using the isobarically constructed FGM the difference is hardly noticeable. With this validation now the intended three-dimensional case is carried out and analysed with respect to stretch and curvature effects.

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Figure 1: The burning velocity at the isotherm of 305 K and at the inner layer, as function of the stretch rate K, for spherically expanding flames, compared with numerical and experimental data.



Figure 2: Laminar flame speed as function of time, DNS (one-step) and DNS-FGM compared to stationary solutions. Left: Results from 1D compressible simulation with one-step chemistry, right: Same result obtained with the appropriate manifold. The numerical code for solving one-dimensional isobaric steady flames is denoted with CHEM1D and dx denotes the constant grid size, also cases with local grid-refinement at a constant number of gridpoints (n) are shown.