Application of FGM to DNS of premixed turbulent spherical flames

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Abstract

The present research deals with the development of a new combustion model in numerical simulations of turbulent premixed combustion. This research is performed in the framework of the application of biogas additions to natural gas as combustibles in domestic and industrial applications. We start from the point of view of detailed calculations. To that end for the aerodynamics we take a DNS code and for the combustion detailed kinetics is taken into account for laminar flames. In order to access practical problems these methods have to be reduced. For this we introduced the Flamelet Generated-Manifolds method in the DNS to obtain accurate chemistry effects at low computational cost. The next steps are the reduction of the aerodynamics by LES and RANS respectively. Then also effects of flame stretch and curvature have to be taken into account.

1 Introduction

The use of bio-fuels is regarded as one of the most promising methods to make a significant contribution to the reduction of the green-house effect. This because it is considered as CO$_2$ neutral, if combined with new strategies to produce biomass. For this reason, the use of bio-gas (mixtures including H$_2$ and CO as combustibles) in gas-turbine combustion for electricity production has gained interest in recent years. In a joint project the Dutch companies NRG and Electrabel Nederland recently started a first assessment of the possibilities to add syn-gas mixtures, produced in a nearby gasification unit, to natural gas for driving their gas-turbine generators.

2 Specific objectives

Combustion in lean premixed gas-turbines predominantly takes place in the flamelet regime and in the thin-reaction zones combustion regime. In the last 20 years a lot of so-called flamelet models have been developed for premixed combustion processes.

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in the flamelet regime. The first and most well-known model is derived by Bray, Libby and Moss [2] by assuming that the flame-front is infinitely thin. A very efficient flamelet model is developed by Peters and coworkers (see [12]) and is based on the so-called G-equation. The G-equation is a kinematic equation which can be used to follow the average position, brush thickness and wrinkling of the flame front. Peters very recently extended the G-equation model for combustion in the thin-reaction zones regime. The model is very efficient since it is not sensitive to the internal structure of the turbulent flame brush. On the other hand, it has the disadvantage that the internal flame dynamics are not taken into account. In spite of these developments, it is still unlikely that all important physics are taken into account in the models available at the moment and it is generally recognized that there is still no reliable model for predicting the turbulent burning velocity. Therefore numerical simulations can not yet be used for the assessment of the stability of the combustion in a gas turbine. Questions, which are not answered are related, for instance, to the influence of counter-gradient diffusion on the flame structure and propagation. As for all Reynolds-Averaged Navier-Stokes (RANS) models of turbulent flows, closure assumptions have to be introduced. For turbulent fluxes one usually invokes a Boussinesq closure hypothesis, assuming that it behaves as a diffusion term. However, in the heart of premixed turbulent flames, this is un-physical because there one mostly encounters fluxes with a counter-gradient diffusive character, de Goey [4]. This might be related to the biased correlations due to gas expansion by the heat release. Another thing is the influence of flame stretch and curvature. The amount of laminar flame wrinkling, described by effective parameters like the flame surface area ratio \( \sigma \) in the G-equation model or the flame surface density \( \Sigma \) in other models, is determined by how effective the flame is stretched and curved by the turbulent structures. Furthermore there is the influence of local flame quenching and ignition and the influence of differential diffusion effects. Our aspiration is to take all these effects into account, but still a lot has to be done to answer these questions. With the use of DNS and employing a well-considered chemical reduction technique a large amount of information concerning these aspects will be accessible.

3 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 [6] 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 by Groot and de Goey [7], in which the theoretical corrections were incorporated. The simulations were carried out with the one-dimensional code CHEM1D, 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. [8] as in figure 1.

![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.](image-url)
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] (the cold case is defined in Vreman et al. [14]). The configuration and results are displayed in figure 2 and figures 3 and 4 respectively. Figure 3 shows the temperature at a cross section at three moments in time and figure 4 isoplanes of $\lambda_2$, an indication of the three dimensional turbulent structures, as defined in Jeong and Hussain [9]. 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 [11] is the flamelet method.

Figure 2: Configuration of the burning mixing layer.

4 DNS-FGM

Figure 3: Temperature at a cross section at $t = 20$, 40 and 80.
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 [11], 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.

5 First results

The FGM method is applied in the DNS to study turbulent spherically expanding premixed flames. For a first validation the FGM technique was implemented in a one-dimensional version of the DNS. The results are shown in figure 5. 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.

6 Future research

The research will logically be continued by extending this DNS-FGM method towards LES. This like the LES-G-equation method of Pitsch and Duchamp de Lageneste [13]. For the volume-
averaging the transport equations is needed for the laminar flamelets as first introduced by Marble and Broadwell [10]. De Goey [3] recently derived a new flamelet model, closely resembling this so-called Coherent Flame Model (CFM). Flame stretch and curvature effects inside the pre-heating zone of the laminar flame structures are taken into account now, but the reaction layer is still regarded as infinitely thin. Following the ideas of Peters, this new CFM model has been extended also to the thin-reaction zones regime ([3], [5]). It appears that the turbulent burning velocity $s_T$ is proportional to $s_L$ and the so-called flame surface density $\Sigma$, being a measure for the amount of flame surface per unit volume. Closure relations are derived for the influence of stretch and flame curvature induced by the turbulent eddies on the flame surface area and for the turbulent fluxes in the averaged transport equations, taking into account gradient and counter-gradient diffusion. The model will be implemented in the numerical code and validated against DNS-FGM of turbulent spherically expanding flames.

The last step towards the treatment of more practical problems is the introduction of the described method of LES-FGM towards RANS. Since the averaging procedure in LES and RANS is more or less analogous this should be not the most difficult step. Although with LES more and more problem will be accessible in the future, still with RANS one is able to obtain quick answers and to perform lots of parameter studies.

7 Conclusions

First results are reported of implementing the chemical reduction technique of FGM into a DNS simulation code. A first one-dimensional investigation shows that with a single controlling variable the laminar burning velocity of a stoichiometric methane air flame can be predicted very accurately. With this method the entire flame structure is known employing a minimal amount of computer time. At the moment the method is used for three-dimensional spherical, premixed and turbulent flames. With this DNS-FGM one is able to validate LES and RANS modeling, which will be developed on the basis of FGM as well.
References


