Numerical Analysis of a Swirl Stabilized Premixed Combustor with the Flamelet Generated Manifold approach

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1 Introduction

In this paper the effectiveness of LES for modeling premixed methane combustion will be investigated in the context of gas turbine modeling. The required reduction of the chemistry is provided by the flamelet generated manifold (FGM) approach of van Oijen [1]. For turbulence-chemistry interactions an algebraic model is used to calculate variations which are used to invoke a pre-assumed pdf, Vreman et al. [2]. The algebraic model has a tunable parameter.

Academic cases have been researched with this model so far and now we assess the potential of the model for turbine combustors, specially the role of the algebraic model, which depends on the appropriate choice related with the tunable parameter. One of the main objectives is to predict the turbulent flame brush at the right location. Since the approach is consistent with a RANS approach, also these kind of simulations (Realizable $k-\varepsilon$) are presented. It follows that the location of the flame brush is predicted too much upstream. This is consistent with a too low value of the parameter, which was also suggested in [2].

The paper starts with a short description of the method and physical problem. Then the manifold is discussed following a presentation of RANS and LES results. The paper ends with conclusions.

2 Combustion Modeling

The flamelet generated manifold (FGM) technique [1] makes use of correlations of species to reduce the number of equations, in the sense that the combustion process

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H. Kuerten et al. (eds.), *Direct and Large-Eddy Simulation VIII*,
ERCOFTAC Series 15, DOI 10.1007/978-94-007-2482-2_51,

is described in terms of a few control variables. The strength of the FGM reduction technique is that the number of independent control variables, starting with a single reaction progress variable c, can be increased for a better description of the chemical phenomena.

At the present lean condition, it is assumed that the progress variable can be sufficiently described by carbon dioxide, CO_2. To check this assumption, thermo-chemistry variables were plotted as function of CO_2 and indeed these variables can be described without ambiguity using just carbon dioxide as the reaction progress variable. Due to the limited space, these plots will not be shown here.

In the FGM technique the real source term can be used, instead of its definition based on empirical correlations as in [3]. The flamelet generated manifold uses a physical laminar source term directly retrieved from a laminar flamelet database generated from a one-dimensional laminar flame calculation. More information about the FGM procedure can be found in van Oijen [1].

If the purpose is to understand the physical aspects of reacting flows in high swirl flow conditions, and therefore combustion occurring in a turbulent flow field, the interactions between chemistry and turbulence must be considered properly. In this approach the flamelet approach combined with a pre-assumed PDF closure method for the chemical source term will be used in order to describe the turbulence-chemistry interactions. For this we will use a commonly used β-PDF function. In a second step, the laminar manifold will be integrated in terms of this function. Now the variables are tabulated as a function of the mean reaction progress variable $\tilde{c}$ and its respective variance $var(c)$. Therefore a transport equation for $\tilde{c}$ and an algebraic equation for $var(c)$ are taken into account, as in Vreman et al. [2]. Here the progress variable is defined as the scaled mass fraction of carbon dioxide $c \sim Y_{CO_2}$ and the variance is taken as

$$var(c) = \frac{a^2 \Delta_k^2}{12} \left(\frac{\partial \tilde{c}}{\partial x_k} \right)^2 \tag{1}$$

An estimation related with the computational time between the current method and cold flow simulations without a lookup, gives an expectation of comparable computing times. This since only one additional transport equation will be solved.

In the FGM approach, chemistry is tabulated *a priori* aside from the flow solution, and therefore a fast look-up procedure to retrieve the thermo-chemical variables from the integrated database, which structured nature is known, is possible.

3 Numerical procedure

The code used here is FLUENT 12.0 which is a commercial finite-volume code. To simulate the flow field for the reacting flow case, the turbulence models used were the Reynolds-averaged Navier-Stokes, RANS (Realizable $k-\varepsilon$) and LES, with subgrid terms modeled using the dynamic Smagorinsky model. The combustor used in the present numerical investigation is referred to as SimVal, as developed by Stakey and Yip [4]. It consists of a slot swirler, a nozzle section and a combustion section

that is encased by a 180 mm diam quartz tube followed by an exhaust section. Further details can be found in [4]. Most of the numerical data obtained were collected using a mass flow rate fixed at 0.045 kg/s, which corresponds to a bulk flow velocity in the nozzle section of approximately 40 m/s.

The three-dimensional computational domain encompassed the region from the exit of the swirl plate to 9 cm into the exhaust section and was comprised of approximately 1.305×10^6 hexahedral cells in a multi block structured grid.

The boundary conditions were considered through the same conditions described in [3], thus the individual slots of the swirl plate at the entrance of the domain were modeled as velocity inlets with specified axial and tangential velocity corresponding to a 30^o flow angle, an inlet temperature $T_{inlet} = 530K$ and $c = 0$ for the scalar (progress variable).

The fluid used was a fully premixed mixture (CH_4/air) at an equivalence ratio $\phi = 0.6$, and the kinematic viscosity was assumed to be constant and based on the preheat temperature.

The time-step used for the LES simulations was 5μs, and the total time of simulation 145.3 ms., which corresponds to approximately 36 flow-through times. The discretization scheme used was a second-order bounded central differencing scheme in space and a second-order backward differencing scheme for the temporal discretization. The scalar equations were discretized with a second-order upwind scheme. We have taken a to be equal to 1.

4 Results

In order to generate the flamelet database for the present case, in a first step the governing laminar free premixed flame is calculated using the package CHEM1D, developed at Eindhoven Technology University. For this case complex chemistry and transport are applied. For the present work, the laminar flame speed, S_L was calculated using the GRI3.0 mechanism which contains 325 elementary reactions between 53 species. It was found that $S_L = 44.5$ cm/s.

In a second step, turbulence-chemistry interactions are taken into account by integrating the laminar database using the β-PDF function. This results in values of the thermo-chemical variables tabulated as a function of c and $var(c)$, e.g., the source term $\dot{c} = \dot{c}(\tilde{c}, var(c))$. The referred steps are shown in Fig. 1 and for both steps, the manifold generation process and its integration in terms of β-PDF, the routines used were developed by Vreman et al. [2].

In order to see the capability related with FGM to simulate combustion in gas turbines, some first results for the turbulent reactive flow field modeled using *RANS* (Realizable $k-\varepsilon$) and FGM as the combustion model were obtained. Considering that the flame front can be related with intermediate species, such as OH, results for the contours of OH mass fractions and also for the axial velocity along the cutting plane through the center of combustor are shown in Fig. 2.

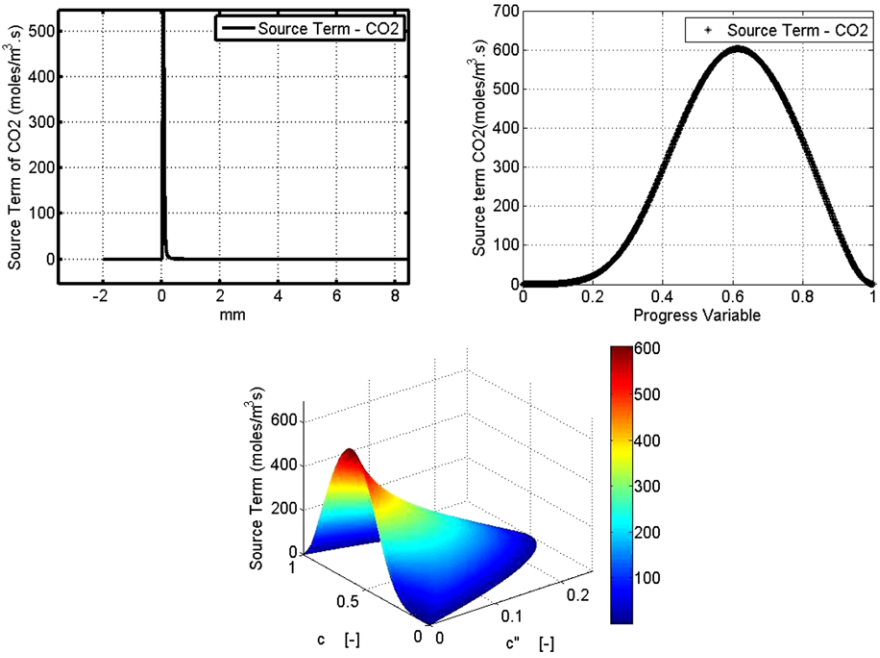

Fig. 1 Upper left: Source term of CO_2 at pressure of 1 bar as a function of the physical space, x. Upper right: Source term of CO_2 as a function of c, $1D$ manifold for the laminar flame (FGM). Lower figure: $2D$ turbulent manifold, source term of CO_2 as a function of c and $var(c)$.

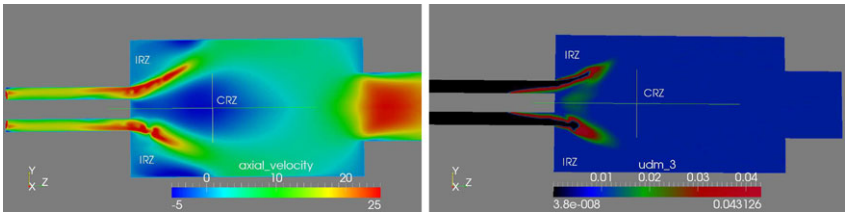

Fig. 2 Results from RANS/FGM. Left: Axial velocity contours. Right: OH contours.

A central recirculation zone (CRZ) and the inner recirculation zone (IRZ) are observed as expected and indicated in the figure. Also, the flame location and shape can be directly observed from the OH contours, and are in agreement with the observed flame shape [3]. Nevertheless, these experimental results show that combustion is located a little further downstream of the combustor dump (entrance) plane.

Considering the intrinsically dynamic nature of the process, LES simulations were also performed in order to verify the effects of unsteadiness and large turbulent scales on the flame front. According to the ratio of flame thickness to the LES filter width, which is of the order of unity, it is possible to conclude that subgrid wrinkling is not important here [2]. Here the flame thickness, $\delta_F \approx 0.6$ mm, is

based on the maximum temperature gradient value computed from the previous $1D$ laminar flamelet calculations. The LES filter width, $\Delta_k \approx 0.75$ mm, is determined from an average of the grid resolution at the combustor dump plane.

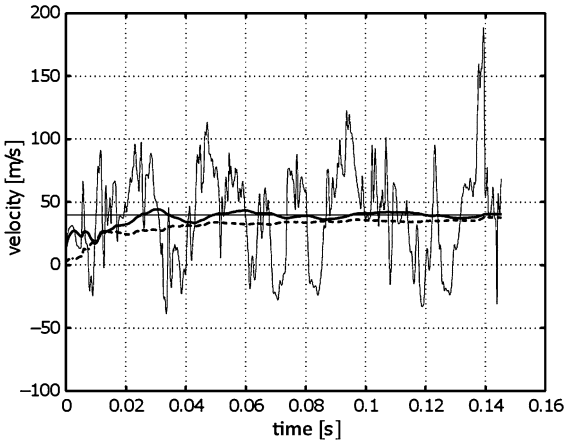

Fig. 3 Axial velocity at a single point at the dump plane, thin line: basic signal, straight drawn thin line: mean axial velocity at the inlet for reference (40 m/s), thick drawn line: running mean, thick dashed line: running rms.

Time series for the axial velocity and for the scalar were monitored in a single point at the combustor dump plane, and the respective cumulative temporal mean and rms of the axial velocity are shown in Fig. 3. It can be visually observed that the results are almost converged with respect to the mean and rms of the axial velocity at the dump plane, being 40.5 and 37 m/s respectively at the end. By analyzing the autocorrelation function we can determine the (Taylor) micro scale to be 0.0015 s and the integral scale to be 0.039 s, which coincides with 97 and 3.7 occurrences in the total simulation time. Note that these values are evaluated from a time series of the LES results. Thus the meaning of these numbers requires careful interpretation. The time history for the progress variable (not shown) shows the unsteady nature related with the mixture alternating between unburnt and burnt. This means that the stabilization of the mean flame comprises the dump plane. In the experiments this is found to be located more downstream. Clearly the present description does not suffice completely.

The effect of the unsteadiness in particular related to the shear layer in the flame region is visualized in Fig. 4. Here it can also be observed that the combustion takes place in a region comprising the dump plane.

The algebraic model for the variance $var(c)$ strongly depends on the parameter a in Eq. (1). In fact the optimum value for the referred parameter is not the same for grids with different filter width, Δ_k [2]. Defining the mean source term in terms of a presumed β-PDF model shows that low values for $var(c)$ implies in large values for the source term, and as can be seen in Fig. $1(c)$ this could be the reason related with the existence of flame also in the upstream of the combustor dump plane.

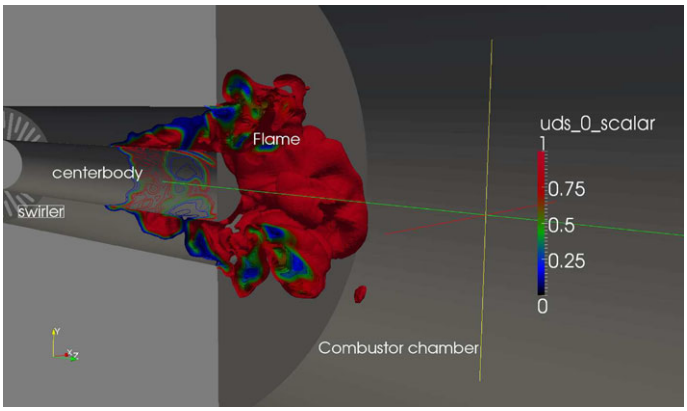

Fig. 4 Cutting plane of a 3*D* instantaneous flame front showing isosurfaces of reaction progress variable, c ($UDS_{scalars}$). The flame zone location and the combustor components are shown.

5 Conclusion

Results concerned with the LES and RANS simulations were obtained for the reactive flow in a gas turbine burner considering the use of FGM as the combustion model.

As an overall conclusion, the simulations performed with FGM shows that through an appropriate look-up procedure, combustion features in gas turbine conditions can be reproduced with a reasonable computational effort. Clearly LES gives much more insight compared to RANS. However, they both give a consistent burning region that is a little too much upstream. To improve the results an evaluation on the parameter of the variance model should be performed. Values approaching $a = 2$ are suggested for comparable cases, [2]. Using a transport equation or a dynamic procedure would also be potential options. In the future non-ideal premixing and heat-loss can be taken into account.

References

1. Van Oijen, J.A.: Flamelet-generated manifolds: development and application to premixed laminar flames. PhD thesis, Eindhoven: University of Technology Eindhoven, (2002)
2. Vreman, A.W., van Oijen, J.A., de Goey, L.P.H., Bastiaans, R.J.M.: Subgrid scale modeling in large-eddy simulation of turbulent combustion using premixed flamelet chemistry. Flow, Turbulence and Combustion, **82**, No. 4, 511–535, (2009)
3. Strakey, P.A., Woodruff, S.D., Williams, T.C., Schefer, R.W.: OH-Planar Fluorescence Measurements of Pressurized, Hydrogen Premixed Flames in the SimVal Combustor. AIAA Journal, **46**, No. 7, 1604–1613 (2008)
4. Strakey, P.A., Yip, M.J.: Experimental and Numerical Investigation of a Swirl Stabilized Premixed Combustor Under Cold-Flow Conditions. J.Fluids Engineering. **129**, 942–953 (2007)