Numerical simulations of a turbulent high-pressure premixed cooled jet flame with the flamelet generated manifolds technique

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Numerical Simulations of a Turbulent High-Pressure Premixed Cooled Jet Flame With the Flamelet Generated Manifolds Technique

In the present paper, a computational analysis of a high pressure confined premixed turbulent methane/air jet flames with heat loss to the walls is presented. In this scope, chemistry is reduced by the use of the flamelet generated manifold (FGM) method and the fluid flow is modeled in an large eddy simulation (LES) and Reynolds-averaged Navier–Stokes (RANS) context. The reaction evolution is described by the reaction progress variable, the heat loss is described by the enthalpy and the turbulence effect on the reaction is represented by the progress variable variance. A generic lab scale burner for methane high-pressure (5 bar) high-velocity (40 m/s at the inlet) preheated jet is adopted for the simulations, because of its gas-turbine relevant conditions. The use of FGM as a combustion model shows that combustion features at gas turbine conditions can be satisfactorily reproduced with a reasonable computational effort. Furthermore, the present analysis indicates that the physical and chemical processes controlling carbon monoxide (CO) emissions can be captured only by means of unsteady simulations. [DOI: 10.1115/1.4029099]

1 Introduction

A predominant part of the world energy demand is obtained by the combustion of fossil fuels. In this framework, gas turbine combustion is one of the most important energy conversion methods today. This is because using gas turbines, large scale, high efficiency, low cost, and low emission energy production is possible. For this type of engines, low pollutants emissions can be achieved by very lean premixed combustion systems. This sort of combustion requires special attention to the balance between emissions, flame stability, and completeness of combustion. In industry, the development of clean and efficient technologies for the combustion process is achieved by a combination of experimental and numerical research. Physical testing is in general extremely expensive, and a great reduction of the costs could be made by maximizing the usage of simulations in the design phase. Experiments are time consuming as well, whereas modern engineering trends tend toward shorter and more efficient design cycles. These reasons, together with the persisting advance in the computer technology, are sufficient to elucidate the phenomenal growth of interest in numerical simulations of reacting flows in the last few decades. Nevertheless, the numerical modeling of combustion systems still represents a very challenging task. The interaction of turbulence, chemical reactions, and thermodynamics in reacting flows is of exceptional complexity. In addition to this, modern lean-premixed high pressure highly turbulent combustion is inherently unstable, requiring therefore additional effort in the modeling.

The objective of this paper is the description of the development, implementation, and testing of a methodology for the simulation of turbulent reacting flows at a reasonable central processing unit (CPU) cost, with application to gas-turbine combustion. To this

end, the FGM chemistry reduction technique [1,2] is implemented and adopted for the simulation of a high pressure confined premixed turbulent methane/air jet with heat loss to the wall. The elevated pressures in combination with high flow velocities and heat loss to the walls demand a superior attention on the modeling, since thinner flames generate stiffer solutions. A generic lab scale burner for methane high-pressure (5 bar) high-velocity (40 m/s at the inlet) preheated jet is adopted for the simulations, because of its gas-turbine relevant conditions. Turbulent, lean premixed flames of different fuels have been experimentally studied in this axis-symmetric gas turbine combustor [3,4]. This research applies the FGM chemistry reduction method coupled with LES and RANS models, in order to predict the evolution and description of the mentioned turbulent jet flame in high pressure (and high Reynolds number) flow conditions, including the important effect of heat loss by conduction to the walls. The results are initially analyzed by comparison with the experimental data, and the effect of heat loss inclusion on the flame characteristics is inspected. Subsequently, an analysis of the accesses to the manifold is performed. This provides useful indications on the direction for improving the manifold storage efficiency in further versions of the FGM technique.

2 FGM

Among numerical combustion models proposed for gas turbine combustion resembling flows, the flamelet concept has attracted great attention [5,6], for both premixed and nonpremixed turbulent combustion. The FGM method [1,2], also referred to as flamelet prolongation of intrinsic low-dimensional manifold (ILDM) [7], is a flamelet-based chemistry reduction method created on the idea that the most important aspects of the internal structure of the flame fronts should be taken into account. In the FGM technique, the course of the reaction is defined in terms of a few control variables, for which transport equations are solved during run-time. And here lies one of the main strengths of the FGM technique, which is that the number of independent control

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variables can be increased for a better description of the combustion phenomena. This means that the accuracy of the method can be straightforwardly extended for the inclusion of heat loss and turbulence, as shown in Sec. 3. The flamelet system is computed in a preprocessing stage, and a manifold with all the information about combustion is stored in a tabulated form. To this purpose a laminar flamelet database is generated from a one-dimensional (1D) flamelet calculation performed with full kinetics and detailed transport. The FGM technique has the admirable advantage of considerably reducing the computational cost of combustion simulations [1,2,8], while keeping the accuracy to high levels. A key advantage of FGM is in fact the capability to predict minor species in a consistent way. The FGM technique has proven to be very accurate for laminar premixed Bunsen flames including heat loss presence [1,9], preferential diffusive effects [10], highly stretched premixed counterflow flames [11], and confined triple flames [12]. This technique performed well also in direct numerical simulation (DNS) of a turbulent expanding flame [13], showing that a single control variable can give accurate predictions on the local mass burning rate. Furthermore, the approach has proven to be appropriate also for the computation of turbulent flames with heat loss [8] as well as for turbulent partially premixed flames [14,15]. However, this technique has been employed only few times to high pressure conditions, and mostly for diffusion flames, e.g., [16,17]. At the best of the authors' knowledge, the application of premixed FGM in combination with heat loss, high pressure, and turbulence has never been studied in literature. In this

research, the FGM chemistry reduction method is applied for the simulation of turbulent methane/air combustion at high pressure conditions with lean equivalence ratio and preheated inlet, with the inclusion of heat loss to the walls. In order to take this into account, in the present implementation the reaction evolution is described by the reaction progress variable, the heat loss is described by the enthalpy and the turbulence effect on the reaction is represented by the progress variable variance.

3 Heat Loss and Turbulence Effects Inclusion in FGM

The FGM technique makes use of correlations of species to reduce the set of equations that describes the whole chemical kinetics. This model retrieves the whole chemistry directly from a laminar flamelet database generated from a 1D steady flat flamelet calculation performed with full kinetics and detailed transport.

In this study, we consider premixed methane/air combustion at high pressure conditions with lean equivalence ratio and preheated inlet. In the present case, the FGM consists of a 3D manifold where the control variables are represented by the (mean) progress variable $\tilde{\mathcal{Y}}$, (mean) enthalpy $\tilde{h}$, and progress variable variance $\tilde{\mathcal{Y}}'^2$. The progress variable $\mathcal{Y}$ quantitatively defines the transition from fresh mixture to burned gases, and it is defined here as the oxygen (O_2) mass fraction. Along the combustion process, the mass fraction of oxygen is continuously decreasing; therefore, this quantity represents an appropriate progress variable. For practical

Fig. 1 Representation of the laminar manifold. (a) Progress variable source term ($\text{kg m}^{-3} \text{s}^{-1}$); (b) temperature (K); (c) density (kg m^{-3}); and (d) enthalpy along the single flamelets composing the manifold.

Fig. 2 The convoluted shape for an adiabatic flamelet. (a) Progress variable source term and (b) CO mass fractions. Laminar (bold curve) and convoluted (dashed) at different levels of variance of the progress variable.

convenience the progress variable is scaled between 0 (fresh mixture) and 1 (chemical equilibrium, which is a function of h).

In the geometry adopted for this simulation, the inlet is considered to be fully premixed, and the pressure constant (5 bar), therefore no additional control variables are necessary to describe these effects. On the other hand, enthalpy is not conserved throughout the domain because of the heat loss to the combustion chamber. In order to take this into account in the tabulation process, the laminar flamelets [1] have to be solved for different values of enthalpy, introducing enthalpy h as a control variable. The procedure for the creation of enthalpy-decreasing set of flamelets might be performed in different ways, but the most straightforward are: (1) decreasing the enthalpy of free adiabatic flamelets by simply diminishing the inlet temperature, with this approach a series of flamelets is computed for different values of $h_{-\infty}$; (2) calculation of burner-stabilized flamelets [1,9], and therefore imposing a certain increasing amount of heat loss to the burner. Here both methods are used in order to have an adequately complete manifold, in fact burner-stabilized flamelets allow to impose very high values of cooling. The application of this procedure is directly recognizable from Fig. 1(d), in which a demarcation line on the enthalpy steps is a clearly visible hint of the switch between the two modes. Nevertheless, it has been proven that the choice of the enthalpy-decrease method for the tabulation procedure has negligible influence on the final result [1,18].

Chemistry is represented by means of the GRI-Mech 3.0 mechanism [19] which contains 325 elementary reactions between 53 species with hydrocarbons up to propane. Unity Lewis numbers

Fig. 3 Overview of the domain by means of a time snapshot of the LES simulation with heat loss. The flame here is represented by an isosurface of progress variable ($\gamma = 0.75$), and colored as function of its source term ($\text{kg m}^{-3} \text{s}^{-1}$).

Fig. 4 Thermal laminar flame thickness and reaction layer thickness as a function of the enthalpy of the flamelet

are imposed along the flamelets, neglecting differential diffusive effects. The underlying reason for this approximation is that at high turbulence levels diffusion of species and temperature is dominated by turbulent mixing [20,21], resulting in an effective unity Lewis number, and allowing a much simpler formulation of the FGM equations [2]. A result of this assumption is that the enthalpy levels are constant throughout the distinct flamelets, because of the even balance between mass and heat diffusion along the reaction.

The peak temperature of the lowest enthalpy flamelet is approximately 1100 K; therefore, an extrapolation is required in the incomplete subcooled region of the manifold. This region is identifiable, e.g., from Fig. 1(d), and consists of the whole triangular area enclosed by the coldest flamelet line $h = h_{\min, \text{flamelet}}$ and the point of minimum enthalpy $h = h_{\min} = -h_{\text{eq}}$. The completion of the data in this zone is very important for cases in which burned gases are cooled, for example. To tackle this problem, a bilinear interpolation is performed between the coldest flamelet and the point of minimum enthalpy. Even if such a procedure represents a coarse approximation, it performs quite well [1]. Fortunately, in most practical cases the cooling takes place in the burned gases, and therefore in the zones approaching the chemical equilibrium line in the manifold. An overview of the resulting manifold can be seen in Fig. 1, where progress variable source term and temperature are represented as a function of the progress variable and enthalpy.

The turbulence-chemistry interaction is taken into account by describing variables in a stochastic way. Locally a variable is described by a probability density function (PDF) defining the probability of occurrence of a certain state. This is, therefore, accounted for by convoluting the laminar database using a β -function shaped PDF [22]. The β -PDF shape has the advantage of including singularities near the end points while being simple to compute. The convolution operation generates an increase of a dimension in the manifold, which finally reaches the number of three dimensions for the present case. The final dimensions for the

manifold are: progress variable, enthalpy, and variance of the progress variable. In Fig. 2, the progress variable source term and the CO mass fraction are represented for different levels of variance of the progress variable, representing the effect of the β -PDF convolution. In this figure, the laminar flamelet (zero variance) is represented by the bold line, while the different dashed lines represent different levels of variance of the progress variable.

During run-time, together with the momentum and continuity equations, the CFD code must solve conservation equations for the mean progress variable $\bar{\gamma}$ and enthalpy $\bar{h}$. These two transport equations [2] adopt a common eddy viscosity turbulent closure model [23]. In addition to the presumed PDF model, a closure is needed for the variance $\bar{\gamma}''^2$. A suitable, and often used, model is the similarity or gradient-based model [22,24]

$$\bar{\gamma}''^2 \approx \frac{a^2 \Delta^2}{12} \left(\frac{\partial \bar{\gamma}}{\partial x} \right)^2 \quad (1)$$

where Δ is the filter width, which is considered to be equivalent to the grid resolution. The parameter a is assumed to be a constant, or determined by a dynamic procedure. For smooth fields and in case of second order discretization, it can be deduced that the value of a should lie between 1 and 2, since $\bar{\gamma}''(1 - \bar{\gamma}) \leq (1/4)$. In this case $a = 1.4$ is used, according to Refs. [22,25].

4 Geometry and Numerical Methods

The geometry consists essentially of a cylindrical confinement. The jet has a diameter $d = 25$ mm and the combustor a diameter of $d_c = 75$ mm, providing flame stabilization by recirculation of hot combustion products. The overall length of the chamber is $22d$. The simulations presented here are performed with an inlet velocity of $v_{\text{in}} = 40$ m/s, inlet temperature of 623 K, fully premixed CH_4 with an equivalence ratio of $\phi = 0.5$ and $p = 5$ bar. The

Fig. 5 Time snapshots of LES with heat loss inclusion, center-plane. (a) Progress variable; (b) enthalpy (J kg^{-1}); (c) temperature (K); (d) hydroxyl mass fractions; (e) progress variable source term ($\text{kg m}^{-3} \text{s}^{-1}$); and (f) progress variable time snapshot at the center-plane of LES with heat loss inclusion with isoline at $h = h_{\min, \text{flamelet}}$. This figure displays the zone of the domain in which the subcooled region of the manifold is accessed.

Fig. 6 Results comparison at different heights. (a) Axial velocity (m s^{-1}); (b) transverse velocity (m s^{-1}); (c) temperature (K); and (d) CO mass fractions. Bold lines represent LES with heat loss, dots RANS with heat loss, and dashes RANS without heat loss inclusion.

corresponding Reynolds number calculated with the inlet diameter is roughly 100,000. The inlet velocity profile is chosen to be parabolic in order to take account of the presence of the walls, and the velocity profile is therefore set in order to conserve the mass flow rate. No synthetic turbulence is added at the inlet flow. Heat losses to the walls are imposed by enforcing a constant temperature $T_w = 623 \text{ K}$ to the walls.

The solver used for the simulations is ANSYS-CFX [26], coupled with the above described 3D FGM implementation. The approaches used for turbulence are LES with dynamic subgrid scale (DSGS) model and RANS RNG $k-\varepsilon$. The LES DSGS model [27] is essentially an extension of the Smagorinsky model [28], as the dynamic model allows the Smagorinsky constant to be calculated locally in space and time. The RANS RNG $k-\varepsilon$ model solves equations for the turbulent kinetic energy k and turbulent kinetic eddy dissipation rate ε , formulated with the renormalization group methodology (RNG) [29]. The algorithm of the software is implicit and pressure-based, and the solver makes use of a conservative finite-element-based control volume method. The solver chosen for the computations of this work is incompressible. For the progress and control variable transport equations, the turbulent Schmidt number is considered to be constant and equal to $Sc_t = 0.7$. In addition to the flow equations, two extra transport equations are solved for FGM: the progress variable and enthalpy

transport equations [8], whereas the variance is algebraically computed.

The 3D mesh of the geometry consists of 3,400,000 hexahedral elements over 3,500,000 nodes, distributed with a refinement in the flame region, where the smallest grid size is 0.2 mm. The combustion chamber is simulated up to the final part of the combustor, with the inclusion of the twin exhaust pipe as visible from Fig. 3.

5 Results

The global structure of the flame is revealed from an instantaneous image of the flame profile in an LES calculation, as represented in Fig. 3. Here an isocontour of the progress variable $\mathcal{Y} = 0.75$ is shown colored as function of the progress variable source term in order to reveal the flame location. The flame base appears highly corrugated and is strongly affected by the instantaneous local flow conditions.

A consideration about the scales involved in the flow and combustion process of the present case must be made in order to ensure the respect of the flamelet hypothesis [30]. An approximation of the turbulent length scales gives an estimate value for the Kolmogorov scale of $\eta \approx 0.02 \text{ mm}$ (calculated taking in consideration values related to zones located in the flame region). In relation to the chemistry, the flame thickness can be calculated based

Fig. 6 (continued)

on the highest value of the temperature gradient along the flamelet, from the chemistry database. A reaction layer thickness can be calculated based on the integral consumption term of the fuel. Considering the flamelet at inlet conditions, therefore without heat loss, the reaction layer thickness can be estimated as $\delta_r = 0.008$ mm. These values confirm the assumption of falling within the thin reaction zone regime with the present simulations. An interesting point can be made by considering those flamelets subject to heat loss. In Fig. 4, respectively, the thermal and reaction layer thicknesses are displayed as a function of the enthalpy of the laminar flamelet. The reaction layer becomes thicker with a decrease of enthalpy (therefore with the increase of heat loss). This indicates a reduced difference of scales between the chemical reaction and the dissipative scales of the flow. In the same way, the thermal thickness is minor at adiabatic conditions. This effect leads to more extended preheating zones on the cooled regions, e.g., next to the wall. The direct consequence of this behavior is that in all cooled regions the flow modeling is additionally crucial in order to have a correct flame location prediction.

Figure 5 displays a series of quantities from a snapshot of the LES calculation, represented at the center-plane. A core flow region is identifiable close to the symmetry axis and close to the inlet. In this zone, the turbulence intensity is relatively low and the axial momentum is very high. The flame stabilizes by means of the recirculation zone that is formed by the sudden expansion past the inlet. Between the core flow and the recirculation zone,

the velocity gradients are such that most of the turbulence is generated in this location [4]. In fact, in the peak of velocity, RMS is reached for regions that are not so close to the dump plane. Closer to the inlet a strong and relatively thin shear layer zone is noticeable. The turbulence level distribution is caused by a combination of these effects: turbulence is first created by the strong shear layer, afterward it is transported and distributed and finally dissipated with the help of the density and viscosity variations due to the chemical reaction. Figure 5(f) shows a time snapshot of progress variable with an isoline at $h = h_{\min, \text{flamelet}}$. The zone of the domain between this isocontour and the walls is accessing the subcooled part of the tabulated data, in which linear assumptions are made in order to complete the manifold (enthalpy is below extinction of the laminar free flame, see Sec. 3). Notably, only a small part of the domain volume lies outside the computed database.

In order to evaluate the difference with standard simulations, which do not include heat loss, a comparison is performed. In Figs. 6(a) and 6(b), a comparison between velocity values of the simulations is displayed, plotted in the center plane at different distances from the inlet. These results show only a very small mismatch between LES and RANS in the axial velocity. However, the transverse velocity shows quite different profiles between LES and RANS. This is due to the small momentum acting on the transverse direction in comparison with the axial one. The mismatch is primarily leading to a different prediction of the

Fig. 7 Hydroxyl mass fraction fields represented at the center plane. Experimental results (top), averaged LES (center), and RANS (bottom). Color bars are omitted for consistency with the experiments; however, the color scale range is defined by the maximum and minimum values locally in each figure.

Fig. 8 CO mass fraction profiles from the LES. Comparison between instantaneous (a) and time-averaged (b) fields at the center plane.

recirculation region extension along the burner. Profiles of temperature and CO mass fractions are, respectively, shown in Figs. 6(c) and 6(d). The major effect of heat loss on the flame behavior is clearly visible from this comparison.

In the experiments of Ref. [3], a most probable flame front contour is obtained by processing the averaged OH signal intensity gradient. A comparison of this experimental values with LES averaged results (with heat loss) reveals a difference in the flame height of +4.9%, while in the RANS (with heat loss) simulations this difference increases to +13.5%. The comparison between experimental data, averaged LES and RANS is shown in Fig. 7. The LES data is here averaged over a period of 10 flow-through times, with a sampling corresponding to the timestep ($4 \mu\text{s}$). This relatively small difference can be explained by the absence of turbulence at the inlet in the simulations. In fact it is shown in Ref. [3] how the inlet turbulence shortens the flame slightly in the present geometry.

A qualitative but engaging comparison of the CO mass fractions for instantaneous LES and averaged LES is displayed in Fig. 8. This image gives an insight on the capability of capturing CO emissions by steady simulations which solve the averaged flow equations. Although the mean quantities provide a sufficient description of global features associated to the characteristics of the turbulent flame structures, the averaged information is insufficient to describe the dynamics of CO emissions. CO production is in fact governed by local scalar fluctuations, and typically not adequately captured by the RANS model as shown from the results of Fig. 6(d). This effect has to be added to the fact that the present implementation of FGM is not considering the diffusion of CO in the direction parallel to the instantaneous flame front.

Fig. 9 Scatter plot representing the accesses to the manifold at a randomly chosen time snapshot, for each combination of the three control variables

This is a typical effect observed when the flame is rapidly cooled down from the wall. This effect is not included in the present FGM implementation, leading to slightly incorrect predictions of CO mass fractions in the region located close to the inlet expansion plane and subject to strong cooling due to the recirculation of burned gases. In order to take this into account, the FGM should be extended with an extra transported control variable which keeps track of CO.

Finally, given that the whole chemistry is stored in the tabulated FGM and retrieved during run-time, it is useful to investigate how

the manifold is accessed during the simulation. Figure 9 illustrates how the tabulated data is accessed at a randomly chosen timestep of the simulation. As expected, a large part of the points are laying in the burned region, because of the considerable extension of the domain. Figure 9(a) shows the scatter plot of enthalpy versus progress variable. From this image, it is noticeable that a vast part of the combustion happens at high enthalpy levels (the active flame regions is mostly far from the wall), and thereafter the exhaust gases are gradually cooled by the walls (right edge of the figure). Additionally, the distribution of the variance of progress variable as a function of the progress variable itself (as given in Fig. 9(b)) displays how the level of variance is rather large along the reaction coordinate, as a result of the fact that the flame is located right in the shear layer. Notably, not all the areas of the FGM tabulated data are actually accessed during run-time. This observation may be exploited to improve the manifold storage efficiency in further studies.

6 Conclusions

The chemistry reduction method FGM is coupled with LES and RANS turbulence models, in order to predict the evolution and description of a turbulent jet flame in high pressure conditions, including the important effect of heat loss to the walls. The method is shown to capture in a coherent way the combustion features, leading to a representative prediction of the flame shape and height. The inclusion of heat loss plays a major role on the flame shape and velocity profiles, indicating a considerable difference on the prediction of the recirculation zones. Notably, high pressure conditions can be simulated with few modifications of the standard FGM technique. Furthermore, the use of FGM as a combustion model shows that combustion features in gas turbine conditions can be reproduced with a reasonable computational effort. The simulation time of the cases performed with heat loss in this paper is on the order of 60 CPU-hours for RANS, and roughly 7000 CPU-hours for LES. This notably low calculation time is due to the use of the FGM reduction model, allowing us to perform broader and more detailed investigations in future works.

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