Large eddy simulation of a partially-premixed gas turbine model combustor

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Abstract

Large-eddy simulations of a dual-swirl gas turbine model combustor (GTMC) are performed. This burner was experimentally studied by Meier et al. (2006), and is operated in the partially-premixed combustion regime. Two different LES-combustion formulations are employed to separately investigate modeling strategies for representing the combustion regime and the turbulence/chemistry interaction. A prior model analysis is conducted to examine the accuracy of describing the turbulent combustion regime inside this burner in terms of premixed or non-premixed flamelet solutions. Modeling results from three different LES computations are compared with measurements for velocity, temperature, and species-mass fractions of CO₂, CO, and H₂. Overall, the simulation results, obtained with a flamelet/progress-variable (FPV) model and a premixed-based filtered tabulated chemistry LES (F-TACLES) formulation, are in good agreement with experimental data. It is shown that the flow-field structure exhibits sensitivity to the representation of the turbulence/chemistry interaction. This is a result of the flame wrinkling at the lifted flame base in the nozzle-near region.

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Keywords: Large-eddy simulation; Gas turbine combustor; Turbulence/chemistry interaction; Flamelet modeling; Turbulent combustion

1. Introduction

The current design of gas turbine (GT) combustion systems is driven by the need for increased power-densities, improved fuel-efficiencies, reduced emissions, and lower maintenance cost. Computational techniques have the potential for providing valuable information for the design of GT combustion systems [1]. Over recent years, remarkable progress has been made in the development of numerical techniques for turbulent reacting flows. In particular, the large-eddy simulation (LES) technique has been demonstrated to provide considerably improved predictions of turbulent reacting flows compared to single-point closure models.

Different LES-combustion models have been developed for application to turbulent reacting flows. However, many of these models have been validated in the context of canonical and unconfined flame configurations, such as jet-flames or simple dump combustors. Furthermore, LES-calculations in complex burner configurations, relevant to realistic GT combustors and
operating conditions, introduce challenges that can be attributed to the lack of experimental data to enable comprehensive model validation, and the geometric complexity and resulting time-consuming mesh-generation. By addressing these issues, several experimental and computational studies have been conducted to establish validation data in GT-relevant combustor configurations. These model combustors are laboratory-scale burners, exhibiting relevant attributes of realistic combustors (such as diffusor, plenum, swirler, and injector assembly). Often, the combustor chamber is modified to provide optical access for non-intrusive diagnostics.

Recent efforts have focused on GT-combustors that operate under premixed conditions. Notable works are LES-computations of the PRECINSTA swirl burner [2–6]. These simulations utilized premixed combustion models to describe the turbulent reacting flow field. Overall, these validation efforts showed that LES results are in good agreement with experimental measurements. Experiments in this burner [7] showed that the incomplete mixing between fuel and oxidizer represents a mechanism for thermo-acoustic instabilities at certain operating conditions. With the exception of one study [6], most computations focused on the stable operating point without considering partial premixing.

Another premixed burner configuration is the TECFLAM [8], which has been developed with the objective to provide validation data for model evaluations. This unconfined burner consists of a movable swirl nozzle with a central bluff body, and the burner assembly is placed inside a co-flowing air stream. Comparisons of simulation results [9–11] with recent measurements [8] showed good agreement for velocities, temperature and major species.

To investigate non-premixed combustion regimes with relevance to aircraft engines, Janus et al. [12] experimentally characterized a model combustor (MOLECULES), consisting of a generic nozzle design with a single swirler assembly. The burner was operated at elevated pressure conditions and with preheated air. LES-computations of this configuration have been performed [13,14]. Although these model assessments were limited to comparisons of the velocity field for reacting operating conditions, these simulations provided valuable information about the flow-field structure and the assessment of modeling strategies.

While considerable efforts have been directed towards burner systems operating in premixed and non-premixed combustion regimes, LES-model validation for partially-premixed operating conditions are not available. In particular, partial premixing can introduce additional challenges for turbulent combustion models, since many formulations rely on a flame-topology-dependent representation to model combustion processes and the turbulence/chemistry interaction.

The objective of this work is to extend previous efforts on the LES-model validation in complex GT combustor configurations. To this end, the DLR gas turbine model combustor (GTMC) is considered, which is operated at partially premixed combustion conditions [15,16]. Moreover, this combustor consists of a dual swirler, representing a more complex configuration than previously considered.

2. Methodology

2.1. Experiment configuration

A schematic of the burner and the computational domain is illustrated in Fig. 1. The injector assembly consists of a central air nozzle, an annular fuel nozzle, and a co-annular outer air nozzle. Both inner and outer air nozzles supply swirling air at ambient temperature from a common plenum. The inner air nozzle has a diameter of 15 mm; the annular nozzle has an inner and outer diameter of 17 and 25 mm, respectively. Non-swirling fuel is provided through three exterior ports. The fuel nozzle is recessed by 4.5 mm below the burner face. The combustion chamber has a square cross section of \( L_x = 85 \) mm in width and \( L_z = 110 \) mm in height. The exit of the combustion chamber is connected to an exhaust tube with a diameter of 40 mm and a height of 50 mm. In the following, \( h \) denotes the axial distance from the bottom of the combustion chamber.

The investigated operating point is “Flame A,” which is characterized by a thermal power of 34.9 kW and a global equivalence ratio of \( \phi_{\text{glob}} = 0.65 \). The corresponding mass flow rates for air and fuel were 1095 and 41.8 g/min, respectively. The burner was operated at ambient
conditions and the inlet temperature was maintained at 295 K. The Reynolds number, based on the minimum outer nozzle diameter, was 58,000. At these inlet conditions, Weigand et al. [15] reported that the flame was acoustically stable but was lifted from the fuel nozzle exit. Due to the confined geometry of the burner, an outer recirculation zone (ORZ) develops in the lower corner of the combustion chamber, and the vortex breakdown leads to the formation of an inner recirculation zone (IRZ).

2.2. LES governing equations

In low-Mach number variable density LES, the instantaneous Favre-filtered conservation equations for mass and momentum are solved. The filter operator introduces a residual stress tensor in the governing equations, which is represented using a Smagorinsky model, and the model coefficient is set to a numerical value of $C_s = 0.17$ [17]. Previous investigations [18] on the same combustor showed that the dynamic Smagorinsky model can result in a different flame shape.

In reacting flows, mass and momentum equations alone are not sufficient to describe the thermodynamic variations due to chemical reactions. Therefore, a combustion model is employed, which relates these thermochemical quantities to a reduced set of reaction coordinates. In the present work, two topology-based LES combustion models are considered for predicting the turbulent reacting flow field, namely the diffusion-based flamelet/progress-variable (FPV) approach [19,20] and the premixed-based filtered tabulated chemistry LES (F-TACLES) model [4,14]. In both models, all thermochemical quantities, denoted by the vector $\psi$, are parameterized by mixture fraction $Z$ and a reaction-progress variable $C$. The progress variable is defined as $C = Y CO + Y CO2 + Y H2O + Y H2$. For LES-applications, this state vector is then discretized using a scheme that is formally second order accurate on unstructured meshes [23]. Time-advancement is achieved through a second order accurate predictor–corrector scheme, and the pressure is obtained as solution to a Poisson equation.

### 2.3. LES combustion models

Since the GTMC operates in a partially premixed combustion mode, this work evaluates the applicability of using non-premixed and premixed combustion models to represent the turbulent reacting flow-field in this burner. Both models utilize a flamelet formulation, in which the thermodynamic state space is parameterized in terms of mixture fraction and a reaction progress variable:

$$\psi = \psi(Z, C),$$  \hspace{1cm} (3)

where $\psi = (T, Y, \dot{\omega}_C, \rho, v, x)^T$. For turbulent combustion applications, this parameterization is expressed in terms of Favre-averaged quantities, which are obtained by integrating Eq. (3) over a presumed joint probability density function (PDF):

$$\bar{\psi} = \int \int \psi(Z, C) \bar{P}(Z, C) dZ dC,$$  \hspace{1cm} (4)
in which \( \bar{P}(Z,C) \) is modeled as \( \bar{P}(Z,C) = \beta(Z;\overline{Z},\overline{Z}^2)P(C|Z) \), and \( \beta \) is the beta-distribution. The closure model for the conditional PDF, \( P(C|Z) \), is dependent on the turbulent combustion model. Details about the combustion models that are considered in this investigation are discussed next.

### 2.3.1. Non-premixed combustion models

The non-premixed flamelet model that is utilized in this work is the FPV approach [19,20]. In this formulation, the flame structure is obtained from the solution of the steady laminar non-premixed flamelet equations [24], which are solved along the entire S-shaped curve. The thermo-chemical state space is then parameterized in terms of \( Z \) and \( C \) to obtain the state-relation (3).

In the FPV-model, the PDF \( P(C|Z) \) is represented by a delta function \( \delta(\overline{C} - C|Z) \). The resulting state-space parameterization of this FPV-model, \( \bar{\psi} = \bar{\psi}(\overline{Z},\overline{Z}^2,\overline{C}) \), requires then the solution of Eqs. (1a)–(1c).

It is noted that this FPV-model does not account for the residual fluctuation of \( C \), which can be significant for events of local flame extinction/reignition and wrinkled flame structures that are not resolved. Therefore, a model extension is considered, in which a beta-distribution is used to provide a statistical representation of the residual fluctuations for the progress variable. In the following, we denote this model as “FPV-Cvar,” and the corresponding state-space parameterization, \( \bar{\psi} = \bar{\psi}(\overline{Z},\overline{Z}^2,\overline{C},\overline{C}^2) \), requires then the solution of Eqs. (1a)–(1d). This model extension has been shown to provide a reasonable representation for moderate extinction conditions [25].

### 2.3.2. Premixed combustion model

The filtered tabulated chemistry for LES (F-TACLES) model [4,14] is the turbulent premixed flamelet model that is utilized in this study. F-TACLES is based on the Flamelet Prolongation of Intrinsic Low Dimensional Manifold (FPI) approach. The manifold \( \psi(Z,C) \) is constructed from 1D laminar unstrained premixed flames that are evaluated for different equivalence ratios within the flammability limit. In application to laminar partially premixed flames, states outside the flammability limit are then interpolated. With application to LES, the 1D premixed flamelet solutions are spatially filtered in the F-TACLES model such that the filtered flame can be resolved on the mesh. As such, \( \psi \) is not obtained from Eq. (4) but is evaluated as

\[
\bar{\psi}(\overline{Z},\overline{Z}^2,\overline{C}) = \int \langle \psi(C|Z) \rangle \beta(Z;\overline{Z},\overline{Z}^2)dZ,
\]

where \( \langle \cdot \rangle \) denotes a one-dimensional spatial filtering operator. The filtering procedure alone is not sufficient to recover the theoretical flame speed. Although Eqs. (1a) and (1c) are solved in the same manner as the non-premixed models, the F-TACLES model utilizes a different transport equation for \( C \).

The non-premixed flamelet model that is utilized in this study. F-TACLES is based on the Flamelet Prolongation of Intrinsic Low Dimensional Manifold (FPI) model [4,14] is the turbulent premixed combustion model such that the filtered flame can be resolved within the flammability limit. In application to laminar partially premixed flames, states outside the flammability limit are then interpolated. With application to LES, the 1D premixed flamelet solutions are spatially filtered in the F-TACLES model such that the filtered flame can be resolved on the mesh.

\[
\nabla \cdot \tau^\text{res}_C = \overline{\Omega_C} + \nabla \cdot \left( (\overline{\xi} - 1)\overline{\rho} \overline{\Delta C} \right),
\]

where the first term on the right-hand side is the thermal expansion term, and the reader is referred to Ref. [14] for details on its evaluation. This model is designed such that the correct flame speed of the filtered flame front is obtained in the limit of vanishing sub-grid scale flame wrinkling. The flame wrinkling model of Charlette et al. [26] is employed in this work.

### 2.4. Prior examination of combustion models

Before applying the combustion models to LES of the GTMC, we will first evaluate the flamelet approximation, and assess whether the experimentally characterized flow field can be represented by either a premixed or a non-premixed combustion model. This analysis is perform through a prior model evaluation, in which experimental scatter data are used as input to the premixed and non-premixed chemistry tables. By considering the scatter data as instantaneous pointwise measurements, this analysis allows to assess the accuracy of the flame-topology representation in the absence of turbulence/chemistry interaction [27–29]. The table evaluation can then be written as:

\[
\psi = \psi(\overline{Z}_{\text{Exp}},\overline{C}_{\text{Exp}}),
\]

in which mixture fraction and progress variable are evaluated from experiments [15,16] using the definition by Bilger et al. [30]. Under the unity Lewis-number assumption, \( Z_{\text{Exp}} \) is consistent with the mixture fraction utilized in both combustion models. Results from this analysis are presented in Fig. 2. To quantify the relative performance of both models, we use the \( L_2 \)-error norm, which is normalized by the maximum value from the measurements. Results from this analysis are presented in Table 1. This analysis shows that both flame representations provide comparable results for temperature. However, the FPI model shows better agreement with measurements for conditional CO2-results, while the FPV model is in better agreement with measurements for intermediate species of CO and H2.

In summary, this prior model examination suggests that both non-premixed and premixed flame representations provide reasonable descriptions of the combustion process in this combustor. This can be attributed to the similarity of the two manifold representations for temperature and
species-mass fractions of CO\textsubscript{2} in the composition space that is accessed by the experimental data. Similar observations were also made by Vreman et al.\cite{31} by considering the partially-premixed piloted jet flame. The present analysis did not assess closure models for the turbulence/chemistry interaction, and it will be shown in Section 4 that these contributions are of greater significance in simulating this burner.

3. Computational setup

Since the plenum and combustion chamber are coupled, the entire burner (see Fig. 1(b)) is discretized using a fully three-dimensional block-structure hexahedral mesh. This base mesh is locally refined to resolve the wall-near region in the swirler and to capture the flow-field separation point in the outer nozzle section. It was noted by Widenhorn et al.\cite{32} that the flow inside the combustion chamber is sensitive to this separation point. Comprehensive mesh-resolution studies have been performed for the non-reacting condition \cite{33} to show that the mesh topology and resolution are adequate for LES. For the reacting case, the elements located in the combustor and swirler region are locally refined such that the maximum edge length is less than 0.7 mm. After the second refinement, the final mesh consisted of 18 million control volumes. The LES-quality, obtainable with this mesh resolution, was assessed using Pope’s criterion\cite{34},

\[ M = \frac{k_{\text{res}}}{k_{\text{r svd}} + k_{\text{res}}}, \]

where \( k_{\text{res}} \) is the resolved turbulent kinetic energy and \( k_{\text{res}} \) is the residual turbulent kinetic energy, which is here estimated from the Smagorinsky model. Results from this analysis are presented in Fig. 3, showing that \( M \) is below the recommended value of 0.2 in the swirler and combustor section. These results also indicate that the walls are not fully resolved, and further refinement is necessary upstream of the swirler.

Boundary conditions at the inlet of the plenum and at the fuel injector are specified in accordance with the experimentally reported data. No
turbulence was imposed at the inlet and a constant inflow profile was prescribed. At the combustor exit, convective outflow boundary conditions were used, and adiabatic no-slip conditions are enforced at all walls of the combustor.

The reaction chemistry is described using the GRI 2.11 chemical model [35], consisting of 227 elementary reactions among 49 species. This reaction chemistry is employed to obtain flamelet solutions under the unity Lewis number assumption. The filter size utilized in the chemistry library generation for the F-TACLES model is constant and is equal to a length of 4 mm. This length scale is approximately ten times the flame thickness for a laminar stoichiometric premixed methane-air flame; it is also approximately six times of the maximum element length in the reaction zone.

4. Results

4.1. Flow-field structure

Statistical results are collected over four flow-through times. The flow-field results of mean axial velocity and mean mixture fraction at the combustor midplane are shown in Fig. 4. These results are obtained using the FPV-Cvar combustion model. The thin black line is the isocontour of the global equivalence ratio \( \phi_{glob} \). These flow-field results show the distinct presence of a “V-shaped” flame. This shape is primarily controlled by a separation point in the expansion section of the outer swirler. At this point, the air stream passing through the outer swirler separates from the combustor walls, resulting in the formation of an outer recirculation zone. The formation of an inner recirculation zone along the centerline is a result of the vortex breakdown. Quantitative comparisons with measurements are also included in Fig. 4(a), and the velocity field in the boxed region on the left corresponds to PIV-measurements that were obtained by Stöhr et al. [36].

4.2. Statistical flow-field results

Comparisons of computed and measured time-averaged axial velocity profiles along four axial sections through the burner are shown in Fig. 5. Overall, good agreement of the simulation results with experiments is obtained. All combustion models provide comparable results, indicating that the hydrodynamic flow field does not exhibit a pronounced sensitivity to the LES-combustion model. Differences between simulations and measurements are primarily confined to the nozzle-near region, showing that all models overpredict the magnitude of the reverse flow along the centerline at locations \( h \geq 10 \) mm. The stronger reverse flow is manifested by an elongated IRZ at the flame base, and can also be seen from the comparison of the computed mean axial velocity field and PIV results in Fig. 4(a).

Comparisons of statistical results for mixture fraction, temperature, and species-mass fractions of CO\(_2\), CO, and H\(_2\) between experiments and simulations are shown in Fig. 6. Overall, the predicted mixture-fraction profiles (first row), obtained from the LES-calculations, are in good agreement with measurements. However, mixture-fraction profiles at the center of the first measurement location (\( h = 5 \) mm) are consistently overpredicted and biased towards fuel-rich conditions. Interestingly, although the predicted
mixture fraction is closer to the stoichiometric value, the predicted temperature profiles are slightly lower than the measurements.

Further downstream at $h = 30$ mm, both the FPV-Cvar model and the F-TACLES model predict temperature and CO$_2$ mass fractions that show better agreement with measurements, compared to the FPV model. This can be attributed to the strong turbulence/chemistry interaction at the flame base, which results in flame wrinkling on the subgrid that is not resolved. These unresolved fluctuations in the progress variable are omitted in the FPV model. However, by considering these effects in the FPV-Cvar model and the F-TACLES method, the agreement improves and both models yield comparable results. This confirms experimental findings by Meier et al. [16] that localized extinction/re-ignition and flame wrinkling can be of importance in this burner. These subgrid scale fluctuations in $C$ are considered through a presumed PDF-closure in the FPV-Cvar model, while the F-TACLES model utilizes a premixed flame wrinkling model to capture this phenomenon.

All simulations utilize an adiabatic combustion model, in which wall-heat losses are omitted. Effects of the heat-losses can be indirectly assessed from the temperature results at the burner face and the side-wall. In particular, for $x \geq 20$ mm at $h = 5$ mm, the computed mean temperature profiles are approximately 150 K higher than the measurements, which suggests that wall-heat losses in regions of extended residence time require consideration. The overprediction of the temperature at near-wall locations seems to extend up to $h = 30$ mm, and experimental quantification of the heat transfer is necessary to substantiate this further.

Despite this highly turbulent condition, model tendencies shown in Section 2.4 are also observable from the different simulation results. Specifically, the premixed model generally predicts

![Fig. 5. Comparisons of mean (left) and rms (right) axial velocity from simulations and experiments at four axial locations through the burner.](image1)

![Fig. 6. Comparison of mean profiles for temperature, mixture fraction, and mass fractions of CO$_2$, CO, and H$_2$ from simulations and experiments at four axial sections through the burner.](image2)
lower mass fractions of CO than the non-premixed models for most measurement locations.

Comparisons at the last measurement location \((h = 90 \text{ mm})\) indicate that the flow is in chemical equilibrium. Predictions of the thermochemical state are identical for all combustion models, confirming model consistency. These results also indicate that CO is nearly fully oxidized to CO_2. In relevance to practical applications it is noted that measurements in the combustor exhaust stream are frequently used for model comparisons. However, comparisons of the equilibrium gas composition only provide incomplete information about the model accuracy in representing transient combustion processes and strong turbulence/chemistry interaction inside the combustor.

4.3. Conditional statistics

To isolate effects of different combustion models on the flame representation, comparisons of mixture-fraction conditioned results are presented in this section. Since the flame structure exhibits a pronounced spatial dependency, this analysis considers two distinct flame regions that delineate the IRZ (corresponding to \(|x| < 8 \text{ mm}\)) and the ORZ \((18 \leq |x| \leq 30 \text{ mm})\). Conditional results for temperature and mass fractions of CO_2, CO, and H_2 at \(h = 15 \text{ mm}\) are shown in Fig. 7. It is noted that for axial locations greater than \(h = 15 \text{ mm}\), the conditional data converge to a narrow region around the global equivalence ratio. Figure 7 shows that the predicted conditional profiles of temperature and CO_2, obtained from the FPV model, are lower than the measurements and the other two simulations in the IRZ. Reasons for this are the reduced reaction progress and the omission of subgrid contributions from the turbulence/chemistry coupling. Conditional results for the outer region (right column of Fig. 7) indicate that the predicted temperature profiles tend to be at the upper range of the measurements, and the measured peak temperature is lower than predicted. Wall-heat losses in the ORZ are likely to be the cause for the lower peak temperature in the measurements. Moreover, the flow near the wall tends to be leaner so that heat losses mostly occur at conditions below \(\Phi_{\text{glob}}\). At this radial location, effects of the turbulence/chemistry interaction appear to be small since all combustion models provide comparable results.

5. Conclusions

Large-eddy simulations of a partially-premixed dual-swirl gas turbine model combustor were performed. In this investigation, different topology-based combustion models were considered to separately investigate the role of the combustion-regime representation (premixed or non-premixed) and the significance of the turbulence/chemistry interaction. Specifically, the diffusion-
based FPV approach [19,20] and the premixed-based F-TACLES model were considered.

Using experimental data, a prior model analysis was conducted to examine whether the experimentally characterized combustion regime can be represented by either a premixed or a non-premixed combustion model. It was shown that the manifolds, generated from premixed and non-premixed flamelet solutions, provide reasonable representations of the thermochemical state space in this burner configuration. This result is in agreement with previous findings for unconfined jet-flame configurations [31].

Following this model evaluation, LES-computations of the GTMC-configuration were performed for the operating point “Flame A,” corresponding to a condition that is acoustically stable but exhibits a lifted flame. The mesh, consisting of 18 million control volumes, was locally refined to resolve regions of strong mixing and areas in the swirler assembly to capture the flow-field separation point. Using Pope’s criterion, the LES-quality was assessed and it was shown that this metric is well below the recommended value in the swirler and combustor. Comparisons of simulation results and measurements showed good agreement and notable differences were confined to the upstream region near the inner swirler. Model predictions for velocity, temperature, and mass fractions of CO2 and H2 were largely insensitive.

An analysis of the temperature results suggests that wall-heat losses reduce the temperature in the outer recirculation region, and temperature measurements in the wall-near region are required to guide further modeling efforts. Through additional studies it was found that this operating point exhibits a supercritical bifurcation that was reflected by the presence of two distinct flame shapes. This bifurcation mode exhibits sensitivities to the resolution in the swirler passage and the subgrid model [18,33]. Further investigations are necessary to quantify this behavior and develop models that capture these transition points.

The hexahedral block-structured mesh is available from the authors.

Acknowledgment

The authors gratefully acknowledge financial support through the NSF CAREER program with Award No. CBET-0844587 and the ONR under Grant No. N00014-10-1-0717. The authors would like to thank Wolfgang Meier and Michael Störh for sharing the combustor geometry and experimental data for model comparisons. This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation Grant No. ASC130004.

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