LES evaluation of PaSR and Extended FGM model on the DLR F400S.3 mGT burner

G. Generini*, A. Andreini*, T. Lingstädt, P. Kutne****
giulio.generini@unifi.it

*Heat Transfer and Combustion group - University of Florence
50139, Via S. Marta 3, Florence, Italy
**German Aerospace Center (DLR)
70569, Pfaffenwaldring 38-40, Stuttgart, Germany

Abstract

The paper approaches a computational evaluation of the DLR micro-Gas Turbine (mGT) burner F400S.3 describing the turbulent combustion through the partially stirred reactor (PaSR) and the Extended Flamelet Generated Manifold (FGM) combustion models. High-fidelity Large Eddy Simulations (LES) were conducted performing a sensitivity analysis on the burner walls' thermal boundary conditions and the combustion model used, comparing the numerical results with the experimental OH*-chemiluminescence distribution. The results showed good agreement regarding the flame shape and reactivity prediction when non-adiabatic thermal boundary conditions were applied at the burner walls and the PaSR model was implemented. On the contrary, the FGM model exhibited underprediction in flame length and reactivity.

Introduction

The utilization of energy carriers, such as hydrogen (H_2), has become increasingly significant in facilitating reliable and demand-centered power and heat supply despite the lack of large-scale infrastructure for hydrogen transport. In this regard, Decentralized Combined Heat and Power (CHP) systems became relevant as they provide high overall efficiency and require only a limited amount of H_2, which can be produced locally [1]. micro-Gas Turbines (mGT) have become the preferred choice for these systems: their low maintenance, high load capability and fuel flexibility have made them an interesting option for CHP generation [2]. However, while the properties of mGTs are well-suited for traditional fuels like natural gas and synthesis gases, the H_2 combustion characteristics present unique challenges that must be carefully evaluated. Therefore, technical challenges need to be addressed to ensure safe and reliable operation. Many studies regarding hydrogen fuelling in mGTs are available in the literature. Calabria et al. [3] were able to experimentally reach 15% H_2 on the AE-T100 Ansaldo Green Tech mGT, underlining the necessity for a burner geometrical redesign to reduce the risk of combustion anomalies onset for higher %H_2. Cappelletti et al. [4] proceeded with a numerical re-design of the burner reaching 100% H_2 computationally while avoiding flashback and self-

ignition. Devriese et al. [5] evaluated, on a different burner, how the fuel nozzle geometry and flame stabilization method influences NO_x emissions. Similarly, Hohloch et al. [6] emphasized how flame stabilization influences the risk of self-ignition and flashback in the mixing zone and how, for H2 fuelled mGT burners, jet-stabilized combustion systems should be preferred over swirl-stabilized ones.
This work aims to investigate the German Aerospace Center (DLR) mGT burner F400S.3 numerically, focusing on a sensibility analysis on the burner walls thermal boundary conditions and combustion model. Initially, a Reynolds-Averaged Navier Stokes Conjugate Heat Transfer (RANS CHT) analysis of the burner was conducted to compute the combustor wall temperature distributions, which were then used as boundary conditions for Large Eddy Simulations (LES). Then, the PaSR and Extended FGM (introducing Stretch and Heat Loss and Gain effects on the flame) combustion models were evaluated on the burner by comparing the CFD results with the experimental OH*-Chemiluminescence data. The PaSR model shows good agreement with the experimental results when non-adiabatic thermal boundary conditions were set at the burner walls. On the contrary, the Extended FGM model underestimates the flame length and lift-off.

Combustion Modelling

Two different turbulent combustion models were implemented within the domain of interest: the Extended Flamelet Generated Manifolds (FGM) and the Partially Stirred Reactor (PaSR) models.
The Extended FGM model [7] is an enhanced version of the traditional FGM approach, including the stretch and heat loss and gain effects on the flame. To achieve this, a correction to the progress variable source term $\dot{\omega}_c$ is performed by multiplying the standard Finite Rate (FR) turbulent source term by a correction factor $\Gamma(\kappa, \psi, Z)$. Γ is tabulated, in a pre-processing step, as a function of the flame stretch κ, the heat loss and gain parameter ψ and the mixture fraction Z. For the sake of brevity, further information regarding the formulation of the Extended FGM model, is provided in [8] for the RANS framework and in [7] for LES. In this regard, additional details concerning κ and ψ formulations can be found in [9].
The Partially Stirred Reactor (PaSR) model [10] is a finite rate chemistry model based on the assumption that the combustion takes place in reactive structures, referred to as "fine scales", which occupy part of the computational cell volume. The PaSR model is generally used for cases where the high dilution levels and the intense mixing between reactants and combustion products lead to a distributed reaction mechanism, resulting in high Reynolds and moderate Damköhler numbers. Additional information regarding the model could be found in [11] and [12], respectively for the RANS and LES frameworks.

Geometry and Numerical Set-up

The DLR F400S.3 burner, shown in Fig. 1, is a reverse-flow jet-stabilized hydrogen-fuelled atmospheric combustor [6]. Air enters the combustor in counter-current with respect to the flue gases flowing between the inner and outer flame tubes. The fuel is divided between two different lines: the pilot line, characterized by a diffusive flame, is used for ignition and a further stabilization of the main line partially premixed flame, properly a jet-stabilized flame. The jet-stabilized combustion system creates a high turbulence level recirculation region, promoting the mixing between the fresh fuel-air mixture and the flue gases before combustion while stabilizing the flame. This is beneficial for hydrogen combustion as it reduces the extension of low-velocity regions and avoid combustion instabilities typical for this fuel.

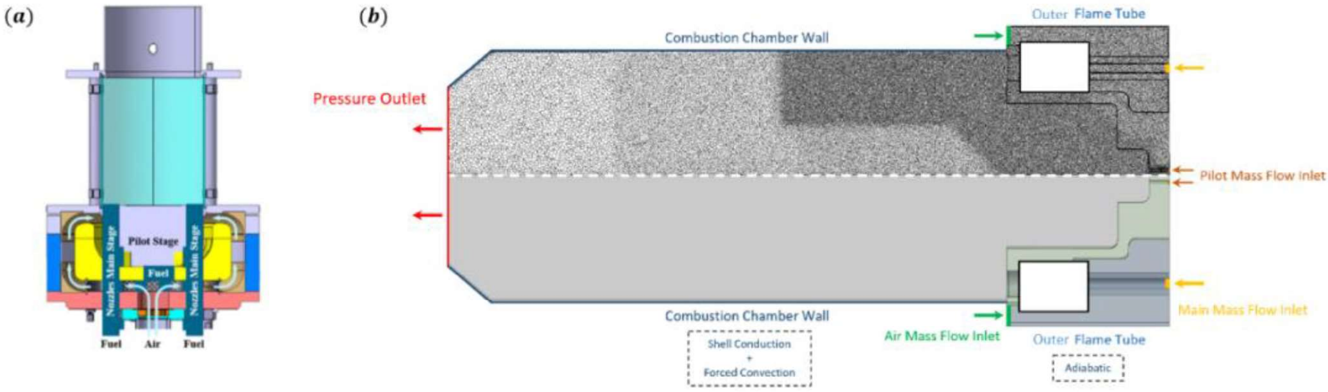

Figure. 1 (a) Experimental Test Case [9]; (b) Computational domain and spatial grid

The Navier-Stokes equations were solved with the pressure-based code ANSYS Fluent 2023 R2, on a 72° sector of the complete burner domain, taking into account the burner periodicity. Initially, to obtain the walls temperature distributions to set as boundary conditions for the LES, a RANS CHT analysis was run on the burner. Here, the combustion chamber wall was simulated as a shell conduction wall, applying the quartz material properties implemented as temperature-dependent polynomials. To take into account the external air flow field cooling effect on the quartz wall, determined by an outlet fan used to promote the flue gas suction, forced convection was modelled. The CHT computational grid, shown in Fig. 1, is composed of approximately 1.4e7 polyhedral cells, obtained by processing an initial hybrid mesh of 24e6 tetrahedral cells with 5 layers of prism adjacent to solid walls. The mesh for the LES CFD analyses was obtained through a similar procedure, neglecting the solid domain in its creation: a polyhedral mesh of about 1.1e7 cells was computed. The chemical reaction mechanism DC1S09, comprising 9 species and 23 reactions, developed by DLR, was used in both the Extended FGM model, for solving of mono-dimensional laminar premixed flamelets and the PaSR model for species transport. For the RANS CHT analysis, the k-ε Realizable with Enhanced Wall Treatment and the COUPLED pressure-velocity coupling scheme were employed, concurrently solving the turbulent combustion using the PaSR combustion model. In the LES context, the effect of unresolved eddies is modelled using the Dynamic Smagorinsky-Lilly formulation which dynamically evaluates the Smagorinsky constant. Turbulent combustion was analysed with both the Extended FGM and PaSR combustion models. Additionally, the SIMPLEC algorithm was adopted for the pressure-velocity coupling with a constant time step of 1e-6 s to ensure a convective Courant number below 5 in the zones of interest. Second-order schemes are used in both space and time using an implicit formulation for this last one. Finally, identical boundary conditions, as shown in Fig. 1, were set for all cases.

Results and Discussion

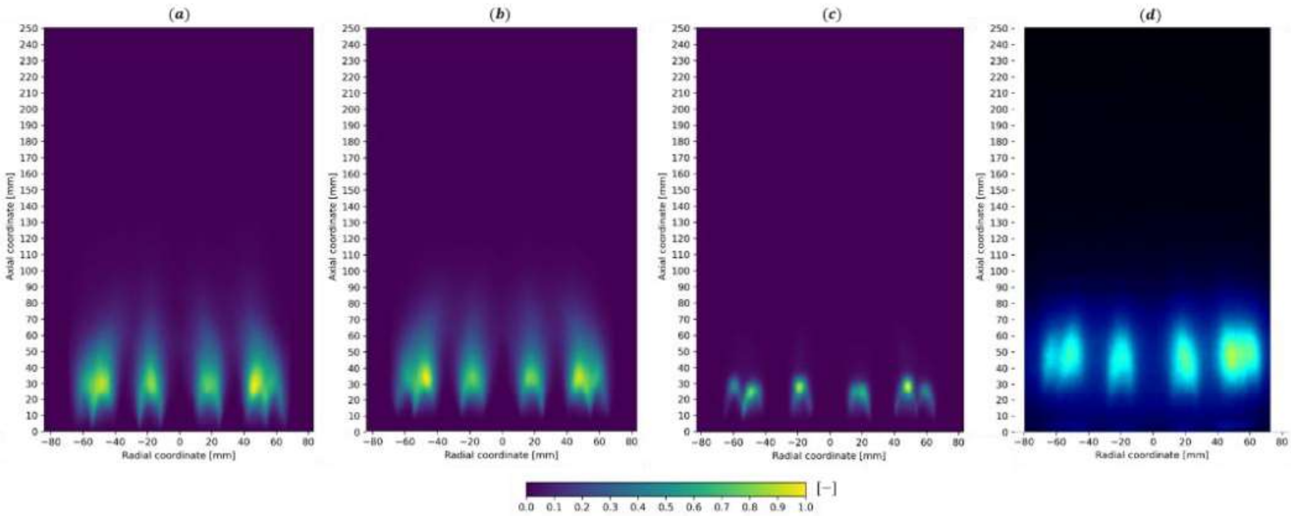

Figure 2 CFD calculated LOS integrated equivalent with (a) PaSR Model with adiabatic walls, (b) PaSR Model with RANS CHT wall temperature distributions, (c) Extended FGM with RANS CHT wall temperature distributions and Experimental OH*-Chemiluminescence (d)

OH*-Chemiluminescence data from experiments (see [6] for further information) were compared with the numerical results by integrating the mean normalized Heat Release Rate (HRR) along the line of sight (LOS) axis to generate the equivalents for comparison with the measured data (Fig. 2). Due to the experimental set-up, the comparison of results is performed only evaluating the partially-premixed main flame.

As mentioned earlier, a RANS CHT analysis was first performed to compute the wall temperature distributions to set as boundary conditions for the LES calculations. Keeping the turbulent combustion model constant (PaSR model) (Fig. 2a and 2b), the thermal boundary conditions introduce flame heat loss, which increases flame lift-off while keeping the flame topology nearly unchanged (Fig. 2b). Despite the improved results obtained by setting non-adiabatic thermal wall boundary conditions, a similar computational setting in the Extended FGM model does not yield comparable results (Fig. 2c). This is mainly due to the fact that the model underestimates the effect of products recirculation on the premixed flame. The model's chemistry tabulation is performed without taking into account the effect of a different oxidant composition determined by the turbulent flow field, which directly brings the pilot and the main flame products onto the premixed flame itself. This is confirmed in Fig. 3a, which provides the laminar flame speed as a function of the mixture fraction for both H2-Air and H2-vitiated-air mixtures at the domain temperature and pressure boundary conditions, computed through the Unity-Lewis and Multicomponent (non-Unity Lewis) transport model. The vitiated-air composition was obtained by computing the species mass fraction on a constant radius surface (shown in Fig. 3b) vertically slicing the combustion chamber, wisely close to where the premixed flame stabilizes, to take into account the influence of both the pilot and main flame products recirculation on the same premixed flame. The normalized mean Heat Release Rate (HRR) distribution on a plane slicing the domain where the premixed flame stabilizes is also shown in Fig. 3b, overlapped with normalized mean radial velocity vectors to better visualize the extension of the recirculation region and thus the path followed by the combustion products.

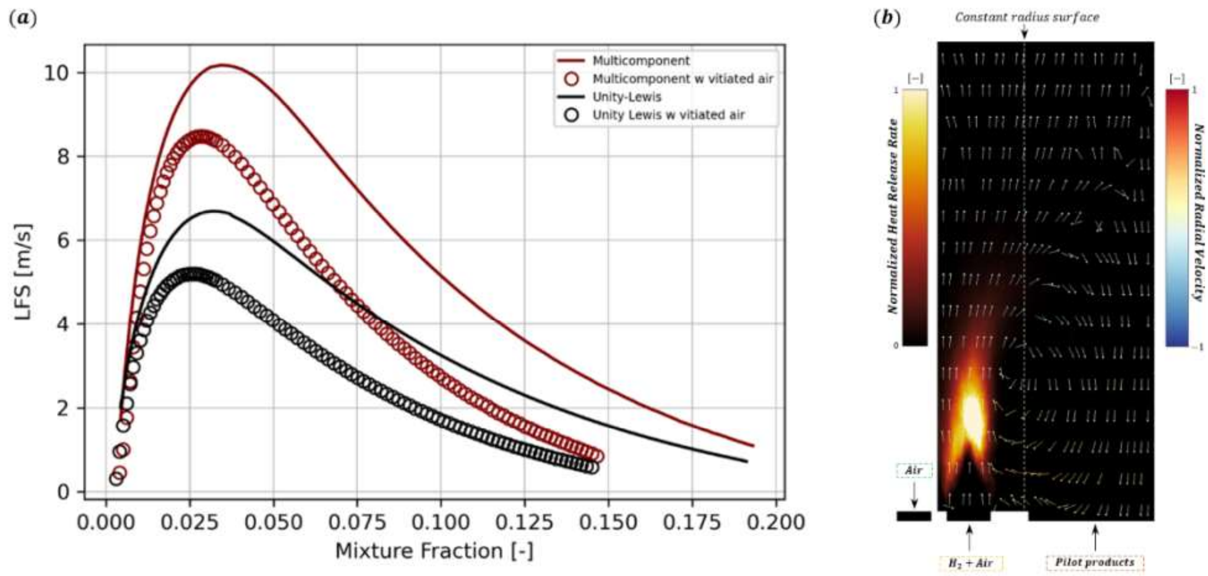

Figure 3 (a) Laminar flame speed as a function of mixture fraction; (b) Normalized mean Heat Release Rate (HRR) distribution overlapped with mean radial velocity vectors.

Conclusions

In this study, the F400S.3 DLR mGT burner was numerically described using Large Eddy Simulations (LES). A sensitivity analysis was performed on the wall thermal boundary conditions and the turbulent combustion model by comparing the Computational Fluid Dynamics (CFD) results with experimental OH*-Chemiluminescence data. Introducing wall temperature distributions obtained from a RANS CHT analysis as thermal boundary conditions for the combustion walls and evaluating turbulent combustion using the PaSR model, the flame characteristics and topology were well captured. The PaSR model is not affected by the limitations of the Extended FGM model, such as its neglect of the recirculation effect of the combustion products on the chemistry tabulation. In this regards, the PaSR model appears to be able to describe adequately the flame characteristics.

References

[1] Maghanki, M. M., Ghobadian, B., Najafi, G., Galogah, R. J., "Micro combined heat and power (MCHP) technologies and applications", *Renewable and Sustainable Energy Reviews*. 28:510-524 (2013)

[2] Banihabib, R., Assadi, M. A., "Hydrogen-Fueled Micro Gas Turbine Unit for Carbon-Free Heat and Power Generation", *Sustainability*.

[3] Calabria, R., Chiariello, F., Massoli, P., Reale, F., "CFD Analysis of Turbec T100 Combustor at Part Load by Varying Fuels", *Proceedings of the ASME Turbo Expo 2015*, Montreal, Quebec, Canada.

[4] Cappelletti, A., Martelli, F., Bianchi, E., Trifoni, E., "Numerical Redesign of 100kw MGT Combustor for 100% H2 fueling", *Energy Procedia*. 45:1412-1421 (2014)

[5] Devriese, C., Penninx, G., de Ruiter, G., Bastiaans, R., De Paepe, W., "The CFD Design and Optimisation of a 100 kW Hydrogen Fuelled mGT", *Proceedings of the ASME Turbo Expo 2020*, Virtual, Online.

[6] Hohloch, M., Lingstädt, T., Kutne, P., "Experimental Analysis of the Hydrogen Capability of a Fuel Flexible Jet Stabilized Syngas Micro Gas Turbine Combustor Under Atmospheric Conditions". *Proceedings of the ASME Turbo Expo* 2023, Boston, USA.

[7] Langone, L., Sedlmaier, J., Nassini, P.C., Mazzei, L., Harth, S., Andreini, A., "Numerical Modeling of Gaseous Partially Premixed Low-Swirl Lifted Flame at Elevated Pressure", *Proceedings of the ASME Turbo Expo* 2020, Virtual, Online.

[8] Klarmann, N., Sattelmayer, T., Geng, W., and Magni, F., "Flamelet Generated Manifolds for Partially Premixed, Highly Stretched and Non-Adiabatic Combustion in Gas Turbines", *54th AIAA Aerospace Sciences Meeting*, San Diego, California, USA.

[9] Generini, G., Andreini, A., Bianchi, E., "Combustion Modelling of the T100 Micro-Gas Turbine burner including the influence of the stretch and heat loss/gain effects on the flame", *Proceeding of the ASME Turbo Expo 2024*, London, England.

[10] Chomiak, J., *Combustion: A Study in Theory, Fact and Application,* Abacus Press/Gorden and Breach Science Publisher, New York, 1990.

[11] Ferrarotti, M., Li, Z., Parente, A., "On the role of mixing models in the simulation of MILD combustion using finite-rate chemistry combustion models", *Proceedings of the Combustion Institute*, 37(4):4531-4538 (2019).

[12] Li, Z., Cuoci, A., Parente, A., "Large Eddy Simulation of MILD combustion using finite rate chemistry: Effect of combustion sub-grid closure", *Proceedings of the Combustion Institute*, 37(4): 4519-4529 (2019).