

NUMERICAL INVESTIGATION OF PREMIXED AND NON-PREMIXED HYDROGEN FLAMES USING LARGE-EDDY SIMULATIONS AND FLAMELET MODELS

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ABSTRACT

A numerical investigation of premixed and non-premixed hydrogen flames is performed with the main aim of assessing the capability of large-eddy simulations and flamelet models to predict the main characteristics of the reactive field. Two different burners are investigated: (i) a premixed bluff body burner fuelled with a lean hydrogen-air mixture ($\phi = 0.4$) and (ii) a non-premixed dual-swirl coaxial injector for which experiments show both anchored and lifted flames for the same global equivalence ratio ($\phi_g = 0.45$). Simulations of the premixed burner are performed using the Flamelet Generated Manifold approach, whereas the two types of flames realized in the non-premixed burner are studied using the Steady Diffusion Flamelet and the Flamelet Generated Manifold. Numerical results are compared with the available experimental data for flow and flame characterization. As far as the velocity field is concerned, the investigated flamelet models have demonstrated capability to properly predict the location and magnitude of the velocity peaks and the shape of the inner recirculation zone in both the premixed and non-premixed cases. Moreover, the computational framework used in this study has demonstrated good accuracy in the prediction of the dynamic behavior of the flow. Regarding the structure of the flame, the models have shown a good capability to predict both the shape of the flame and the location of regions of high-intensity heat release rate. The present investigation offers a comprehensive assessment of large-eddy simulations and flamelet methods in the prediction of the behavior of two archetypes of hydrogen flames of industrial interest. The assessment shown here can provide support for the choice of methods to study cases with increased level of complexity.

Keywords: Turbulent Combustion, Large Eddy Simulation, Hydrogen Combustion, Bluff-body, Swirling flames, Premixed combustion, Non premixed combustion, Flamelet

tion, Flamelet

NOMENCLATURE

Roman letters

d	Diameter [mm]
$\dot{m}$	Mass flow rate [kg/s]
T	Temperature [K]
p	Pressure [Pa]
Z	Mixture fraction
c	Normalized progress variable
LHV	Lower heating value [MJ/kg]
PFR	Product formation rate [1/s]
HRR	Heat release rate [$W\ m^{-3}$]
$TFUP$	Triple flame upstream propagation
Greek letters	
μ	Molecular dynamic viscosity [Pa s]
χ	Scalar dissipation rate [s^{-1}]
ρ	Density [$kg\ m^{-3}$]
$\beta - PDF$	Beta Probability Density Function

Dimensionless groups

σ	Prandtl/Schmidt number
Pr	Prandtl number
Sc	Schmidt number

Superscripts and subscripts

H_2	Hydrogen stream
air	Air stream
u	unburnt mixture
b	burnt mixture
amb	Ambient conditions
SGS	Sub-grid scale property
t	Turbulent property
$\sim$	Favre filtered

1. INTRODUCTION

Hydrogen is one of the most promising fuels to decarbonize the energy and transportation sectors, due to the zero-carbon

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emissions produced by its direct combustion. However, hydrogen combustion remains very challenging due to the very different physical and chemical properties of this fuel compared to standard fuels used in propulsion and power generation. For instance, compared to widely used hydrocarbons, hydrogen is characterized by very high molecular diffusion, low activation energy and fast laminar burning velocity [1–3], which make not straightforward the use of hydrogen in combustors originally designed to operate with hydrocarbon fuels. In addition, the high reactivity of hydrogen may result in high NO_x emissions and risk of flashback if mitigation measures are not adopted. Therefore, to enable an extensive use of hydrogen, new combustion technologies must be developed together with an improved understanding of the combustion characteristics of hydrogen in flames of practical interest. In the context of transition to a zero-carbon economy, it is also important to remark that production and storage of hydrogen still have their own challenges, which must be addressed together with the development of combustion technologies [4]. Lean premixed flames, where the temperature of the reacting region can be controlled through the composition of the mixture, are still considered a reference technology for the limitation of emissions, especially NO_x. However, when hydrogen is used, the risk of flashback can greatly increase [5]. Therefore, new technologies have been proposed such as microjets, which limit the risk of flashback by injecting hydrogen through an array of non-premixed jets. This non premixed configuration consists of injecting hydrogen through an array of high-momentum jets of submillimeter radius [6]. The objective of micro-mixing is to separate fuel and oxidizer prior to injection, therefore avoiding flashback, and at the same time enabling a quick mixing in the vicinity of the injection plate to ensure a quick transition to a premixed regime [7]. Therefore, to develop reliable and safe combustion systems it remains necessary to develop fundamental understanding of hydrogen flame behavior in the two extreme configurations of fully premixed and non premixed combustion. Premixed flames occur when fuel and oxidizer are thoroughly mixed before entering the combustion chamber. The advantages of premixed flames include efficient and uniform combustion, reduced emissions, and greater control over combustion processes, making them ideal for applications requiring low (or controlled) release of pollutants. The main drawbacks of premixed flames include susceptibility to flame instability, limited operating range due to flammability limits, and potential for flashback or combustion oscillations under certain conditions [8], making them more difficult to control than non-premixed flames. Also, some pollutants are more prone to appear in premixed conditions than non-premixed ones. On the other hand, non-premixed flames allow greater flexibility in adjusting fuel-oxidizer ratios for specific combustion requirements, wider operating ranges, and reduced risk of flashback, offering versatility in various combustion applications. However, non-premixed flames present potential for incomplete combustion leading to higher emissions of pollutants, increased sensitivity to variations in flow conditions, and the need for complex control mechanisms to maintain flame stability [9]. Different types of geometries can be used to help in the stabilization of the flame and to reduce the emission of NO_x such as bluff bodies and swirling flows [10]. In particular it has been

noticed that the latter produce an IRZ (Inner Recirculation Zone) of the hot gases that enhances flame stabilization and serves as a source of energy for the incoming reactants. The interaction between swirling flows and a reacting field determines the flame shape and location. It has been observed that changes in the geometry and flow characteristics (e.g., swirl number) could lead to different anchoring points of the flame. An example is provided by Marragou et. al, who report an analysis of the transition from an anchored to a lifted flame [11]. This phenomenon is relevant because a lifted flame operates mainly in a partially premixed regime, leading to a substantial reduction in NO_x. To gain further understanding over the combustion process of hydrogen for flames of practical interest and to validate models used for the prediction of the flame behavior, three different test cases have been recently released by the International Workshop on Measurement and Computation of Turbulent Flames (TNF) [12]. For all these test-cases, measurements on pure hydrogen premixed and non premixed flames are provided. Numerical simulations nowadays play crucial role in the design of combustion units, e.g. to downselect burner configurations or conduct optimization analysis. In the context of flames characterized by a high level of unsteadiness and anisotropy (e.g., vortex breakdown phenomena in swirling flows), large-eddy simulations offer the possibility to provide an accurate prediction of the mixing field. The presence of a reacting field also introduces scales related to chemistry. When turbulence-chemistry interactions are important (low *Da* flames), a time-resolved description of the flame structure with detailed chemistry is needed for a reliable characterization of the flame behavior [13]. If the chemical time scales are small compared to the time scales associated to turbulence, a flamelet description of the flame structure has been proven to provide accurate predictions. Moreover, if the flame is working in a flamelet regime, complex detailed combustion mechanisms can be used to build a flamelet library without increasing the computational cost. Although numerical methods have been extensively assessed and validated for hydrocarbon fuels, when it comes to hydrogen, which is characterized by a significantly different behavior compared to hydrocarbon fuels, such detailed validation of the numerical tools has not been performed yet. Aniello et al. [14] have investigated the non premixed flame studied at the Institut de Mécanique des Fluides de Toulouse (IMFT) using the Dynamic Thickened Flame model (DTFLES) showing that the thickened flame model is able predict the behavior of the two types of flames thereby investigated. The same test rig was investigated by Ballotti et al. [15] where a dynamic thickening strategy for high-fidelity computational fluid dynamics was developed for the analysis of multi-regime combustion. Some works using flamelet models are also available on the premixed flame studied at the Norwegian University of Science and Technology (NTNU) [16, 17], even though the operating conditions used in these works are different and there are also small differences in the geometry used by the authors. In the latter, different CH₄/H₂ - air mixtures have been investigated with LES including the use of various models for the reaction rate source term. The same burner was also investigated in [18–20] using a thickened flame model to study the phenomena associated with ignition. With the overall aim of further assessing the ability of established models to predict

the characteristics of hydrogen flames of industrial interest, the objectives of the present work are to: (i) investigate the capability of flamelet models to predict the flame structure and the behavior of the flow of premixed and non-premixed hydrogen flames; (ii) assess the capability of flamelet models to provide a reliable prediction of the dynamic behavior of the flame, including lift-off. The first objective is addressed by comparing the experimental measurements of the mean axial and radial velocities against the corresponding time-averaged results obtained by the LES. In addition, available experimental data on OH-Chemiluminescence and OH-PLIF are respectively compared with the time averaged results of Heat Release Rate (HRR) and OH mass fraction in order to study the flame structure. The second objective is addressed by comparing the available measurement on the dynamic behavior of the flow such as the RMS of the axial and radial velocity fluctuations against LES results. A flame that exhibits lift-off has also been selected to assess the capability of the selected models to predict lifted flames. The paper is structured as follows. First the configuration and investigated cases are described. Then, the numerical methods and computational setup are presented. This is followed by the presentation of results and their discussion. A summary of the work and main conclusions close the paper.

2. CONFIGURATION AND INVESTIGATED CASES

Two different test cases are investigated in this work. The first case, which will be referred to as ‘NTNU’ case, is a bluff-body premixed flame. The second case, which will be referred to as ‘HYLON’ case, is a non-premixed swirled flame. These two test cases allow us to cover the most common flame and flow configurations, therefore providing a comprehensive assessment of the models investigated here. The two geometries are presented in detail in the following sections.

2.1 NTNU case

The premixed flame configuration studied at the Norwegian University of Science and Technology (NTNU) consists in a bluff-body stabilized burner. A schematic of the geometry is shown in Fig. 1. The conical bluff body has a diameter $d_b = 13$ mm and half-cone angle $\alpha = 45^\circ$. The hydrogen-air mixture is injected through an annular duct surrounding the bluff-body holder. The external diameter of the inlet duct is $d_i = 19$ mm, whereas the bluff-body holder has a diameter of 5 mm. The burner downstream of the bluff body operates with no confinement. Therefore, the flame develops in a free environment at ambient pressure and temperature.

The bluff body’s holder is centered by a set of three transversal cylinders (of diameter 2 mm each) that are placed at a distance of 65 mm upstream of the bluff-body top surface. The location of these cylinders is sufficiently far upstream not to affect the flame dynamics [21–23]. Regarding the operating conditions, the hydrogen-air mixture is injected at room temperature, $T_{amb} = 25^\circ\text{C}$. The mass flow rate of hydrogen and air are equal to $\dot{m}_{H_2} = 2.92 \times 10^{-5}$ kg/s and $\dot{m}_{air} = 2.258 \times 10^{-3}$ kg/s, respectively. The equivalence ratio is kept constant at $\phi = 0.4$; the laminar flame properties at this equivalence ratio are reported in Table 1. Given that $LHV = 120$ MJ/kg, the hydrogen flow rate supplied to the rig results in a thermal power of the burner equal to $P_{th} = 3.5$ kW.

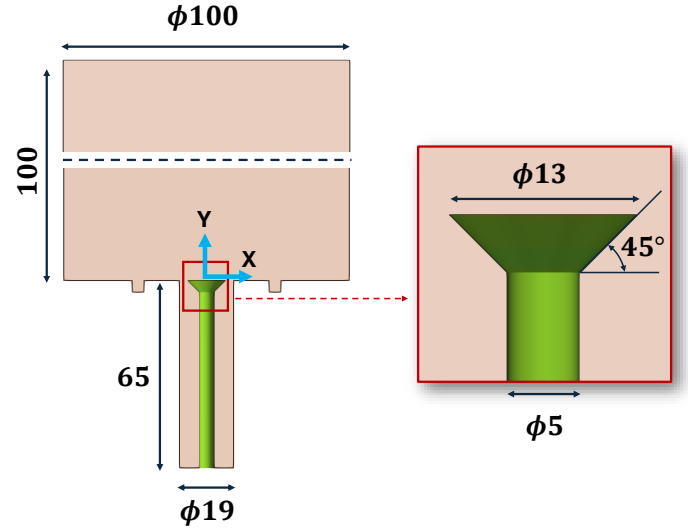


FIGURE 1: SCHEMATIC OF THE NTNU PREMIXED HYDROGEN BURNER: THREE-DIMENSIONAL VIEW OF THE BURNER ASSEMBLY (LEFT) AND VERTICAL CROSS SECTION PASSING THROUGH THE BLUFF-BODY AXIS (RIGHT). ALL DIMENSIONS ARE REPORTED IN MM.

TABLE 1: LAMINAR FLAME PROPERTIES AT $\phi = 0.4$. FROM LEFT TO RIGHT: ADIABATIC FLAME TEMPERATURE, LAMINAR FLAME SPEED, LAMINAR FLAME THICKNESS AND CHEMICAL TIME SCALE.

ϕ	T_{ad} [K]	s_l [m/s]	δ_l [m]	τ_f [s]
0.4	1434	0.21	6.5×10^{-4}	0.0031

2.2 HYLON case

The non-premixed flame studied in this work is the HYLON burner (HYdrogen LOW NOx) dual swirl injector investigated at the Institut de Mécanique des Fluides de Toulouse (IMFT). A schematic of the configuration is shown in Fig. 2.

The burner is characterized by two swirling coaxial ducts for the separate injection of hydrogen and air with dimension $d_{air} = 18$ mm and $d_{H_2} = 4$ mm, respectively. The combustion chamber has the following dimensions: side $h_c = 78$ mm, length $L_c = 150$ mm and outflow diameter $d_o = 73$ mm. A gap of $z_i = 4$ mm between the exit of the hydrogen nozzle and the entry of the combustion chamber enhances the mixing between the two streams. Two different operating conditions are investigated in this work: Flame A, which is attached to the hydrogen nozzle, and Flame L which is lifted above the fuel injector. The flow and fuel quantities for these operating conditions are reported in Table 2.

3. METHODS

3.1 LES-Flamelet Model

Numerical simulations are performed using the large-eddy simulation (LES) approach coupled with tabulated flamelets. Following the flamelet approach, it is assumed that the turbulence

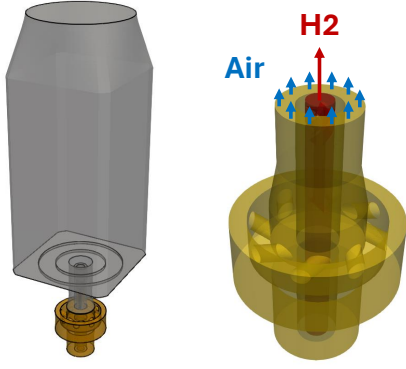


FIGURE 2: SCHEMATIC OF THE HYLON NON-PREMIEXED HYDROGEN BURNER: THREE-DIMENSIONAL VIEW OF THE BURNER CONFINEMENT (LEFT), AND THREE-DIMENSIONAL VIEW OF THE INJECTOR (RIGHT). HYDROGEN AND AIR ARE INJECTED THROUGH TWO SEPARATE DUCTS (YELLOW FOR AIR AND RED FOR HYDROGEN). BOTH STREAMS ARE SWIRLED AND BEFORE THE COMBUSTION CHAMBER THERE IS A ZONE TO ENHANCE THE MIXING BETWEEN THE TWO STREAMS.

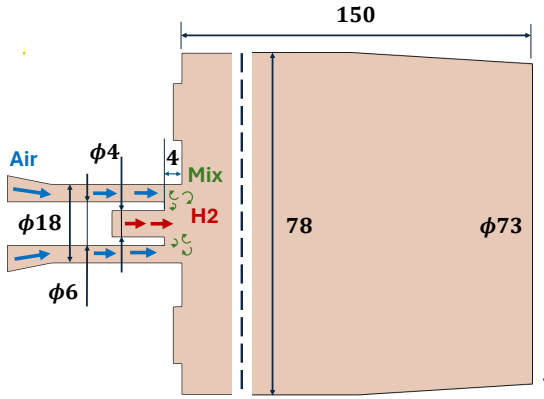


FIGURE 3: CROSS-SECTION OF THE HYLON BURNER PASSING THROUGH THE AXIS OF THE INJECTOR (ALL DIMENSIONS ARE IN MM).

does not affect the flame structure, which can be represented by pre-computed laminar flames. Progress variable and mixture fraction are used to identify the local burning state and composition of the mixture. The effect of turbulence on the flame characteristics is modelled with a presumed-pdf approach, computed from the filtered values of the progress variable and mixture fraction and their sub-grid scale variances. Pre-tabulated flamelet libraries are built using a Beta Probability Density Function ($\beta - PDF$). In this work, two different flamelet models are used and evaluated:

- The *Steady Diffusion Flamelet* (SDM), where the control variables are the filtered mixture fraction, $\tilde{Z}$, its sub-grid scale variance, $\tilde{Z}''^2$, and the stoichiometric scalar dissipation rate $\tilde{\chi}_{st}$ (i.e., the scalar dissipation rate at $Z = Z_{st}$).

TABLE 2: HYLON OPERATING CONDITIONS FOR THE TWO FLAMES INVESTIGATED IN THIS WORK.

Flame	$\dot{m}_{air}$ [kg/s]	$\dot{m}_{H_2}$ [kg/s]	T_{air} [K]	T_{H_2} [K]	P_{th} [kW]	p [Pa]
A	2.41×10^{-3}	3.2×10^{-5}	298	298	3.89	101325
L	6.03×10^{-3}	8.0×10^{-5}	298	298	9.73	101325

The stoichiometric scalar dissipation rate is computed from the mixing field solution with the following algebraic closure:

$$\tilde{\chi}_{st} = C_{\chi} \frac{\mu_{sgs} + \mu}{\rho \sigma_t} |\nabla \tilde{Z}|^2, \quad (1)$$

where C_{χ} is a constant with a default value of 2 [24], μ and μ_{sgs} are respectively the molecular and the sub-grid scale viscosity, ρ is the density, σ_t is a constant turbulent Prandtl/Schmidt number and $\tilde{Z}$ corresponds to the filtered mixture fraction. The stoichiometric scalar dissipation rate is included in the tabulation using a delta-function PDF. Therefore, the filtered value of a generic variable, $\tilde{\alpha}$, can be obtained as:

$$\tilde{\alpha}(\tilde{Z}, \tilde{Z}''^2, \tilde{\chi}_{st}) = \iint \alpha(Z, \chi_{st}) P_Z(\tilde{Z}, \tilde{Z}''^2) P_{\chi}(\chi_{st}) dZ d\chi_{st} \quad (2)$$

- The *Flamelet Generated Manifold* (FGM), where the control variables used for the flamelet tabulation are the filtered mixture fraction, $\tilde{Z}$, its sub-grid scale variance, $\tilde{Z}''^2$, the filtered progress variable, $\tilde{c}$, and its sub-grid scale variance, $\tilde{c}''^2$. In the FGM approach, the filtered value of a generic variable, $\tilde{\alpha}$, is pre-tabulated as:

$$\tilde{\alpha}(\tilde{Z}, \tilde{Z}''^2, \tilde{c}, \tilde{c}''^2) = \iint \alpha(Z, c) P_Z(\tilde{Z}, \tilde{Z}''^2) P_c(\tilde{c}, \tilde{c}''^2) dZ dc. \quad (3)$$

The mean reaction rate in the filtered progress variable transport equation is modelled as proposed by Zimont [25].

Both these flamelet models are implemented by default in ANSYS FLUENT R23.1, which is the software used for the present investigation. As far as the combustion mechanism is concerned, the reduced GRI MECH 3.0 with 10 species and 29 reactions was used in both simulations [26]. Since experimental measurements of OH^* are available for the HYLON burner, the OH^* reactions have been added to the combustion mechanism following Ref. [27]. The look-up tables were built integrating the results obtained from 1D laminar flame simulations using ANSYS Fluent.

3.2 Numerical Setup

In the following, the computational domain and numerical setup of the two test cases are discussed in detail. The computational domains and mesh were built using ICEM CFD R19.

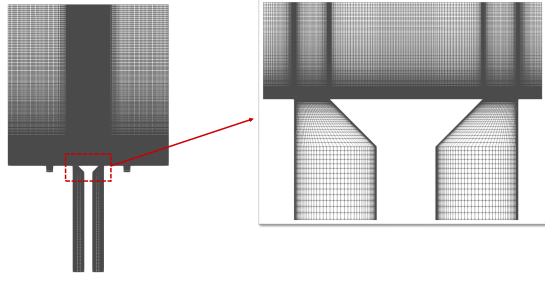


FIGURE 4: NTNU COMPUTATIONAL DOMAIN. A STRUCTURED MESH WAS USED WITH A REFINEMENT OF THE GRID NEAR THE WALL IN ORDER SOLVE THE BOUNDARY LAYER.

TABLE 3: BOUNDARY CONDITIONS USED FOR THE INVESTIGATION OF THE NTNU CASE.

NTNU Boundary Conditions	
H2+Air Stream	Mass Flow Inlet
Bluff Body	No-Slip Wall
Inlet Duct	No-Slip Wall
Plate	No-Slip Wall
External Surface	Pressure Outlet
Outlet	Pressure Outlet

3.2.1 NTNU case. The computational domain starts immediately after the set of three cylinders that were placed 65 mm upstream of the bluff-body plane. The open atmosphere above the bluff-body is modelled as a cylinder with diameter $d = 100$ mm and height $h = 100$ mm. This is schematically shown in Fig. 4. The domain was discretized with a grid of 8 million hexahedral cells. The mesh in the boundary layers was built in order to keep the y^+ value at all walls below 1.0. Table 3 reports the boundary conditions used in the computations. The respective boundaries are indicated in Fig. 5. Figure 5 also reports the different locations that were used to compare numerical simulations with experimental data. Green lines correspond to locations that were used for both cold and reactive flow simulations, while blue and red lines indicate locations where only cold or reactive flow, respectively, were assessed against experiments. A mass flow rate of $\dot{m} = 0.00229$ kg/s was imposed at the mixture stream inlet, as a result of the sum between $\dot{m}_{air}$ and $\dot{m}_{H_2}$ (see Table 3). The mixture fraction value imposed at the mixture inlet, $Z = 0.0125$, was calculated from the experimental equivalence ratio ($\phi = 0.4$). Both cold and reactive flow simulations were performed. A time step of 1×10^{-7} s was chosen to keep the Courant number below unity. The FGM model was selected for the reactive flow. The look-up table was built using premixed freely propagating 1D laminar flames.

To assess the capability of the simulations to capture the flow structures, time-averaged and RMS of axial and radial velocity components were compared with the experimental data. The capability of the model to predict the flame structure was assessed

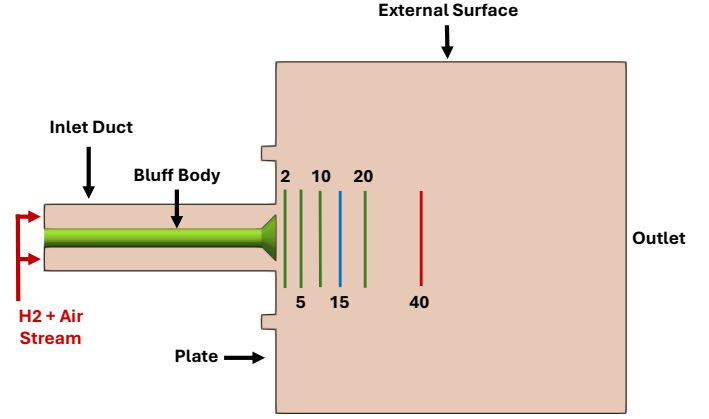


FIGURE 5: BOUNDARY PATCHES AND LOCATIONS AT WHICH COMPARISON BETWEEN EXPERIMENTAL DATA AND COMPUTATIONS IS PERFORMED FOR THE NTNU TEST CASE. GREEN LINES CORRESPOND TO LOCATIONS USED FOR BOTH COLD AND REACTIVE FLOW SIMULATIONS, WHILE BLUE AND RED LINES ARE LOCATIONS USED FOR THE ASSESSMENT OF ONLY COLD OR REACTIVE FLOW SIMULATIONS, RESPECTIVELY.

through comparisons with experimental data on OH-PLIF and OH*Chemiluminescence. These two quantities were compared with the time-averaged OH mass fraction and the time-averaged heat release rate (HRR), respectively. The HRR was calculated as proposed by [17]:

$$HRR = \rho PFR LHV_{H_2} \tilde{Z}, \quad (4)$$

where ρ is the density of the gas, PFR is the Product Formation Rate [1/s], LHV_{H_2} is the lower heating value of hydrogen and $\tilde{Z}$ is the filtered mixture fraction.

The suitability of the mesh for LES simulations was verified by checking whether at least 80% of the turbulent kinetic energy was resolved [28]. The resolved spectrum of turbulent kinetic energy was calculated as follows using the C elik criterium [29]:

$$LES_{IQ} = \frac{1}{1 + 0.05 \left(\frac{\nu + \nu_{SGS}}{\nu} \right)^{0.53}} \quad (5)$$

where ν is the kinematic viscosity and ν_{SGS} is the kinematic subgrid viscosity. Results for the reactive flow simulation are shown in A, which demonstrate that more than the 80% of the kinetic energy is solved throughout the computational domain.

3.2.2 HYLON case. The computational domain for the HYLON test case comprises the burner geometry downstream of the hydrogen and air injection location. This domain was discretized with a structured mesh of 5 million cells, shown in Fig. 7. Swirler ducts were not included in the computational domain. The velocity profiles assigned at the air and fuel inlets were computed by performing preliminary RANS simulation of the injector only, discretized with an unstructured mesh of

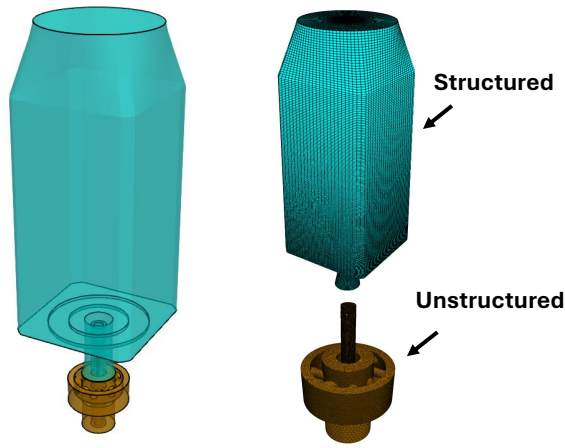


FIGURE 6: GEOMETRY DECOMPOSITION FOR THE HYLON CASE AND MESHING STRATEGY.

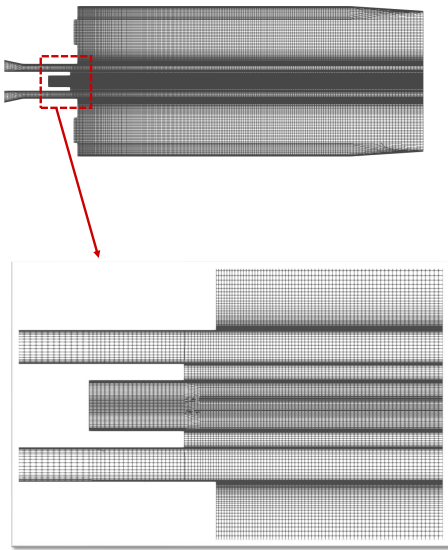


FIGURE 7: HYLON COMPUTATIONAL DOMAIN

tetrahedral cells (see also Fig 6). The preliminary RANS simulation of the injector was carried out with the $k-\omega$ SST turbulence model. Profiles of x , y , and z components of the velocity and of turbulent kinetic energy k and specific dissipation rate ω were then extracted and assigned as inlet conditions for the burner.

For the simulation of this burner, the SDM model was used for Flame A, whereas the FGM model was used for Flame L. This choice was made because, as explained by [11], the lifted flame evolves mainly in the partially premixed regime where the FGM model performs better than an approach for non-premixed flames only. Large-eddy simulations were carried out using a time step of 1×10^{-7} s. Table 4 reports the boundary conditions. The corresponding boundaries are labeled in Fig. 8.

Comparison with experiments was performed in terms of time-averaged and RMS values of axial and radial components of the velocity. Figure 8 shows the locations where experimental data

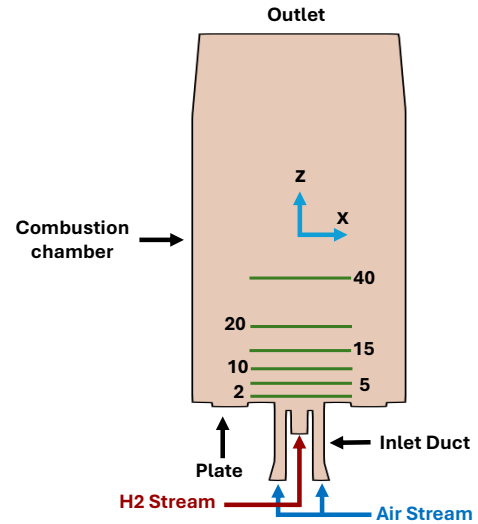


FIGURE 8: BOUNDARY PATCHES AND LOCATIONS AT WHICH COMPARISON BETWEEN EXPERIMENTAL DATA AND COMPUTATIONS IS PERFORMED FOR THE HYLON TEST CASE.

TABLE 4: HYLON BOUNDARY CONDITIONS

HYLON Boundary Conditions	
H2 Stream	Velocity Inlet (profile)
Air Stream	Velocity Inlet (profile)
Combustion Chamber	No-Slip Wall
Inlet Duct	No-Slip Wall
Plate	No-Slip Wall
Outlet	Pressure Outlet

were extracted for both the cold and reactive flow simulations. Moreover, measurements of OH^* chemiluminescence are available to study the flame structure. This set of data was compared with the time averaged OH^* mass fraction obtained from LES. An analysis of the resolved and modelled turbulent kinetic energy in the reactive flow simulation is reported in A. This analysis demonstrates that more than the 80% of the kinetic energy was solved throughout the computational domain.

4. RESULTS AND DISCUSSION

4.1 NTNU case

Figures 9 and 10 show the comparisons between the time-averaged and RMS values of the axial and radial velocity components at different axial positions. Simulations are in good agreement with the experiments. In particular, simulations are able to predict the peaks of the axial and radial velocity components as well as the RMS of their fluctuations. Also, by comparing the axial velocity of the cold flow and reactive flow cases (see Fig. 10), it is possible to note the increase in the extent of the IRZ. Concerning the behavior of velocity fluctuations, the LES is able to predict the evolution of the RMS of both the axial and radial velocities in the cold flow. However, in the reactive flow, RMS of the radial velocity in the shear layer is over-predicted. The over prediction is also significant in the central region at the height of 20 mm.

The flow fluctuations in the reacting simulations are the results of the coupling between the flow dynamics and the changes in density and composition due to chemical reactions. Accurately reproducing velocity fluctuations in reacting flows is challenging. These results demonstrate that the modelling framework investigated here is able to predict the time-averaged behavior. However, refinements may be necessary to further improve the prediction of fluctuations. Figure 11 shows time-average velocity and RMS of velocity fluctuations in a cross-section passing through the axis of the bluff-body. Numerical results are compared with experiments. As already discussed, the time-averaged velocity components are predicted with good accuracy. However, the RMS of the velocity fluctuations tends to be over-predicted both in the shear layers formed at the edges of the bluff-body and annular duct and in the central region of the domain (downstream of the bluff-body). This behavior was also observed in other investigation of bluff-body burners, e.g., Ref. [30].

Regarding the prediction of the flame structure, Fig. 12 shows a comparison between the experimental data of OH* Chemiluminescence and the time averaged normalized HRR. Figure 12 also shows a comparison between the experimental data for OH-PLIF and the time averaged OH mass fraction. The flame predicted by the simulation appears thinner than the experimental data. It is worth noting that the FGM model in its basic formulation implemented in ANSYS FLUENT does not include the effects of stretch. As discussed by Klarman et al. [31], the shape of the flame can be more accurately predicted if these effects are included in the construction of the look-up table. Future work will involve implementing more accurate models that can account for the effects of stretch and differential diffusion models in order to compare the different approaches.

To further investigate the flame characteristics, the Takeno Index was used to differentiate regions of the flame burning in premixed or non premixed mode. Fig. 13 shows the instantaneous contour plot of the flame index. A value of +1 indicates premixed combustion, while a value of -1 corresponds to non-premixed combustion. The combustion regime is fully premixed over the entire flame region and this allows the FGM model to perform at its best since the look-up table was built with premixed flamelets.

4.2 HYLON case

Figures 15 and 16 show the comparison between experimental and numerical velocity components for cold and reactive flows, respectively. Results show that the model is able to predict the axial and radial velocity components in both operating conditions. This means that the shape of the IRZ as well as the swirled motion are captured by the model. The RMS of the velocity fluctuations is also well predicted both for the radial and axial components of the velocity. These results suggest that the LES framework used in the present study is able to capture the variations of the velocity flow field between the cold and reactive flow, caused by the thermal expansion of gases. Table 5 reports a comparison between the experimental values for the averaged temperature of the gases at the outlet of the burner and the time-averaged temperature predicted by LES simulations performed in the present work and results by Aniello et al. [14]. The LES-flamelet model used in the present work results in overprediction of the temperature

TABLE 5: MEAN TEMPERATURE AT THE BURNER'S EXHAUST FOR THE HYLON TEST CASE. MEAN TEMPERATURE OF GASES AT THE OUTLET: T_{exp} INDICATES THE TEMPERATURE MEASURED IN THE EXPERIMENT; T_{CFD} ARE THE RESULTS FROM THE SIMULATIONS PERFORMED IN THE PRESENT WORK; T_{TF} INDICATES THE RESULTS OBTAINED BY ANIELLO ET AL. [14].

Flame.	T_{exp} [K]	T_{TF} (Aniello et al.) [K]	T_{CFD} [K]
A	1138	1010 (-11%)	1338 (+17%)
L	1280	1100 (-16%)	1246 (-2.6%)

for Flame A, whereas for Flame L the time averaged temperature is remarkably close to the experimental value.

To investigate the local presence of multiple flame regimes, the instantaneous contour plot of the Takeno Index is shown in Fig. 14. Unlike the NTNU case, the flame here is characterized by multiple regimes, including both premixed and non-premixed combustion. This complexity makes the flame characteristics more difficult to predict since the look-up table can only be constructed using either premixed or non-premixed flamelets. The presence of multiple combustion regimes on the flame front may lead to less accurate predictions due to the use of the table [32]. Moreover, this effect, combined with the limitations of the flamelet models, such as the use of a presumed PDF function and reduced accuracy near walls [33], could result in an overestimation of the temperature, as observed for the attached flame. In this study, enthalpy losses were not considered due to the lack of thermal boundary conditions from the experiments, particularly at the injector lip of the fuel stream. Additionally, radiative heat transfer was neglected.

As far as the flame structure is concerned, Fig. 17 shows a comparison between measurement and numerical predictions of OH*. Overall, the model is able to correctly predict the shape of the visible flame, reproducing the regions of high heat release rate along the shear layer. The absence of OH* in the recirculation region of Flame A is also well predicted. For Flame L, the model is able to predict a thicker flame, the larger area of high heat release rate further downstream of the bluff-body, as well as the presence of OH* in the area above the bluff-body. Some discrepancies between experiments and numerical simulations are observed in terms of extent of the area with OH* presence and angle between the burner axis and the line where a greater release of OH* is observed, see Fig. 17. Note that the present numerical results are in agreement with the LES-TFUP simulations by Marragou et al. [11], demonstrating that the prediction of the experimental flame angle is a challenge for numerical simulations.

As discussed in [11], a lifted flame can move upstream only if two conditions are met: (i) a flammable mixture fraction line Z_0 , that represent the edge flame propagation line, between the flame and the injector exists and (ii) the mixture fraction Z_0 is located, from the flame to the injector lip, in a zone where the projection of the local velocity u_t along this line is lower than its propagation velocity s_d . The edge flame speed s_d on the Z_0 line is calculated as follows:

$$s_d = s_l^0 \left(\frac{\rho_u}{\rho_b} \right)^{1/2} \quad (6)$$

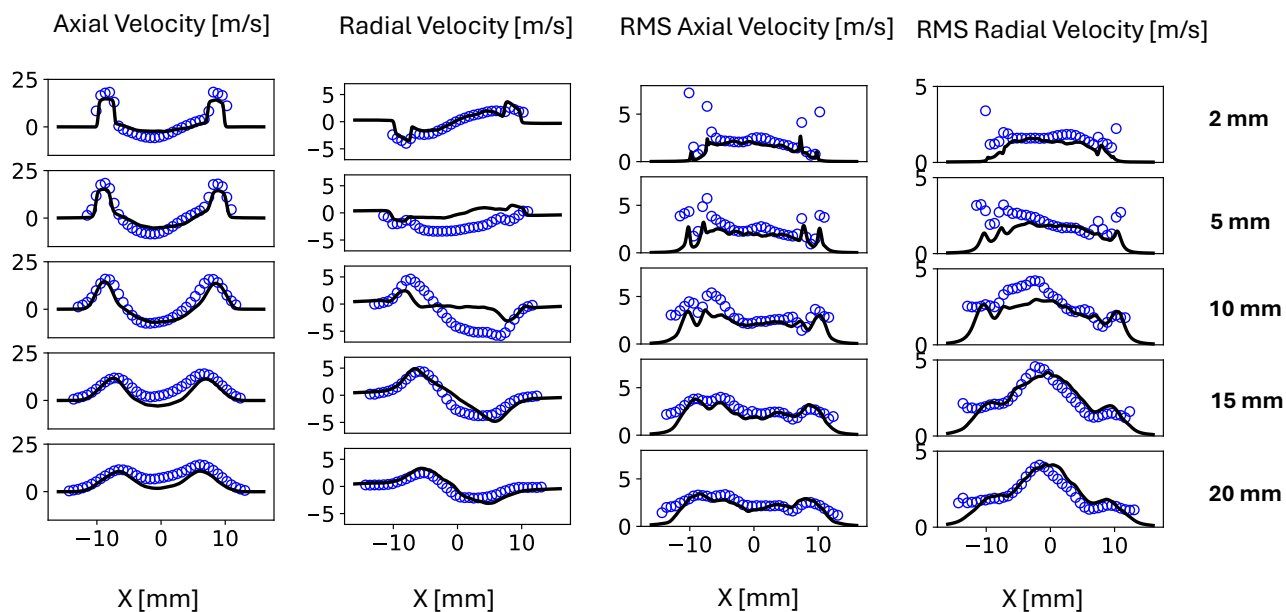


FIGURE 9: NTNU COLD FLOW SIMULATION (LES: —, EXP: ○)

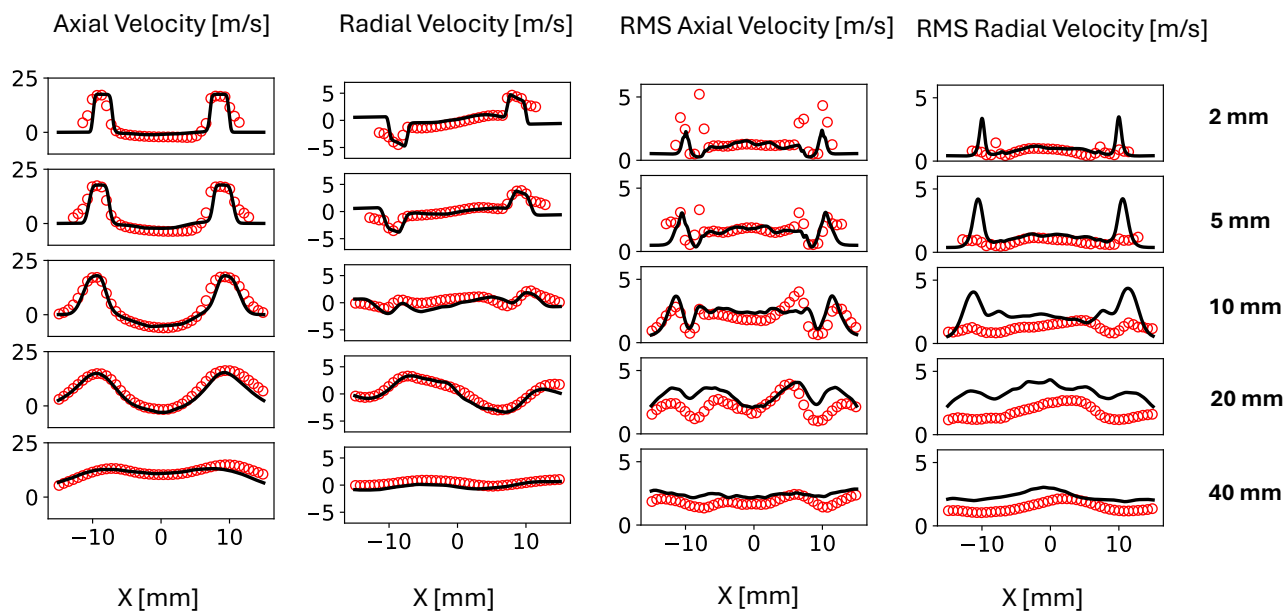


FIGURE 10: NTNU REACTIVE FLOW SIMULATION (LES: —, EXP: ○)

where s_l^0 is the maximum laminar flame speed and ρ_u/ρ_b is the volumetric expansion ratio of the gas through the flame for Z_0 . The mixture fraction Z_0 in most cases is equal to Z_m associated to the maximum laminar burning velocity and maximum triple flame speed. These quantities have been calculated with Cantera [34] using a freely propagating hydrogen flame and the reduced

GRI mech 3.0 (9 species 29 reactions).

First, the laminar flame speed was calculated for different compositions of the mixture to calculate the maximum laminar flame speed obtaining a value of 3.14 m/s as shown in figure 18.a. From the value of maximum laminar flame speed and the mixture fraction at which this value occurs ($Z_m = 0.048$), another freely

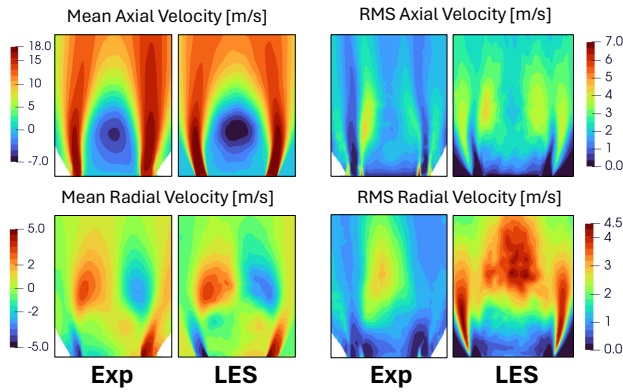


FIGURE 11: CONTOUR PLOT OF TIME AVERAGED AND RMS VELOCITIES COMPARED TO THE EXPERIMENTAL DATA.

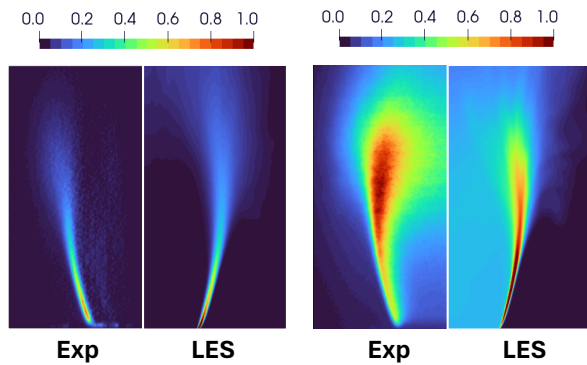


FIGURE 12: LEFT: COMPARISON BETWEEN OH* CHEMILUMINESCENCE AND TIME-AVERAGED NORMALIZED HRR. RIGHT: COMPARISON BETWEEN OH PLIF AND TIME AVERAGED OH MASS FRACTION.

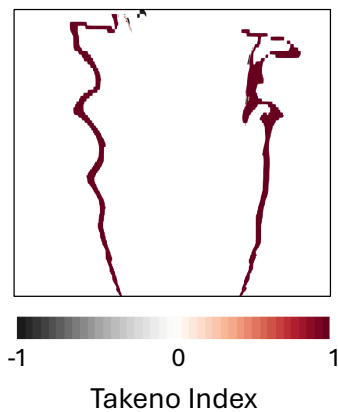


FIGURE 13: INSTANTANEOUS CONTOUR PLOT OF THE TAKENO INDEX. A VALUE OF +1 INDICATES PREMIXED COMBUSTION, WHILE A VALUE OF -1 CORRESPONDS TO NON-PREMIXED COMBUSTION.

propagating flame at the mixture fraction Z_m was simulated to find the volumetric expansion ratio of the gas ρ_u/ρ_b , obtaining a value of 5.91 as highlighted in figure 18.b. The edge flame speed

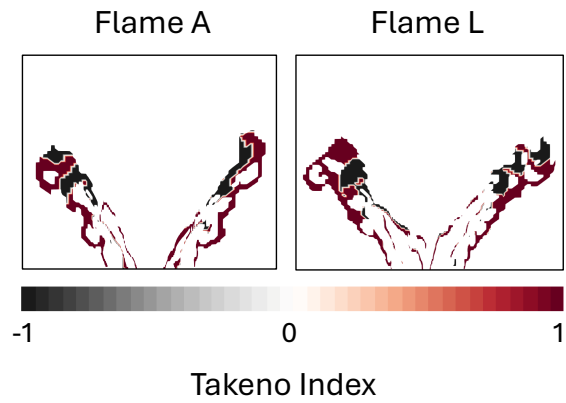


FIGURE 14: INSTANTANEOUS CONTOUR PLOT OF THE TAKENO INDEX FOR BOTH THE FLAMES A (LEFT) AND L (RIGHT). A VALUE OF +1 INDICATES PREMIXED COMBUSTION, WHILE A VALUE OF -1 CORRESPONDS TO NON-PREMIXED COMBUSTION.

s_d is at this point calculated and equal to 7.39 m/s. Once this value is determined, it becomes possible to verify whether the conditions for obtaining a lifted flame are satisfied. As shown in Fig. 19, the purple line, representing the isocontour of Z_m , intersects the TFUP region for Flame A but lies entirely outside the TFUP region for Flame L, in accordance with condition (ii) of the TFUP model. This calculation illustrates how the LES predictions align with experimental observations regarding the occurrence of an anchored or lifted flame.

5. COMPUTATIONAL COST

The simulations were conducted on a high-performance computing cluster using 8x32-core Intel Xeon Platinum 8358 (Ice Lake) CPUs. The computations were initially conducted using Reynolds-Averaged Navier–Stokes (RANS) simulations before transitioning to Large Eddy Simulation (LES). Time-averaged data were collected over four flow-through times for each case, after the influence of the initial RANS solution was fully dissipated. The estimated computational cost was approximately 40,000 core-hours for the NTNU case and 30,000 core-hours for the HYLON case.

6. SUMMARY AND CONCLUSIONS

Premixed and non-premixed hydrogen flames were investigated using LES and flamelet models with the main aim of assessing the capability of the simulations to predict the flame structure and characteristics of the reacting field in two different regimes. Numerical results show that the flamelet models are able to capture with good accuracy both the turbulent field and flame structure.

In the premixed configuration, results demonstrate that the LES-FGM approach provides a good prediction of the flow field measured in the experiment. The agreement between experimental and numerical data is better in the reactive case compared to

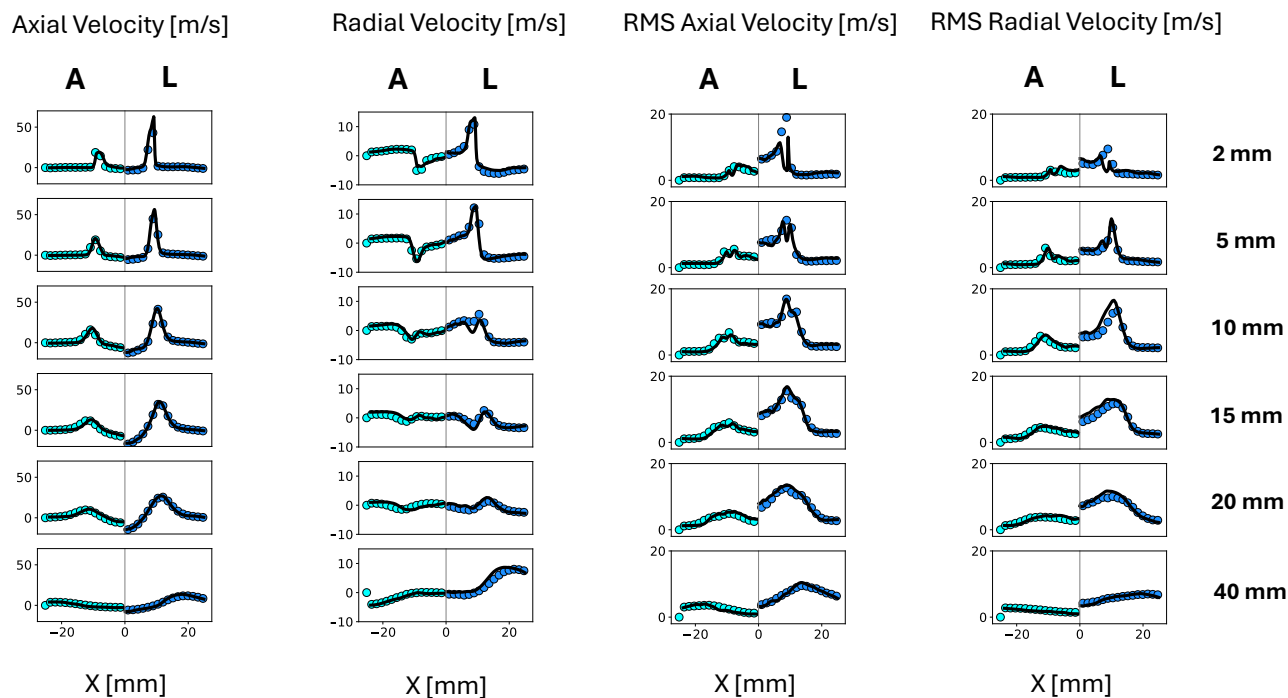


FIGURE 15: HYLON COLD FLOW SIMULATION OF BOTH A (LEFT) AND L (RIGHT) CONFIGURATION (LES: —, EXP: CIRCLES).

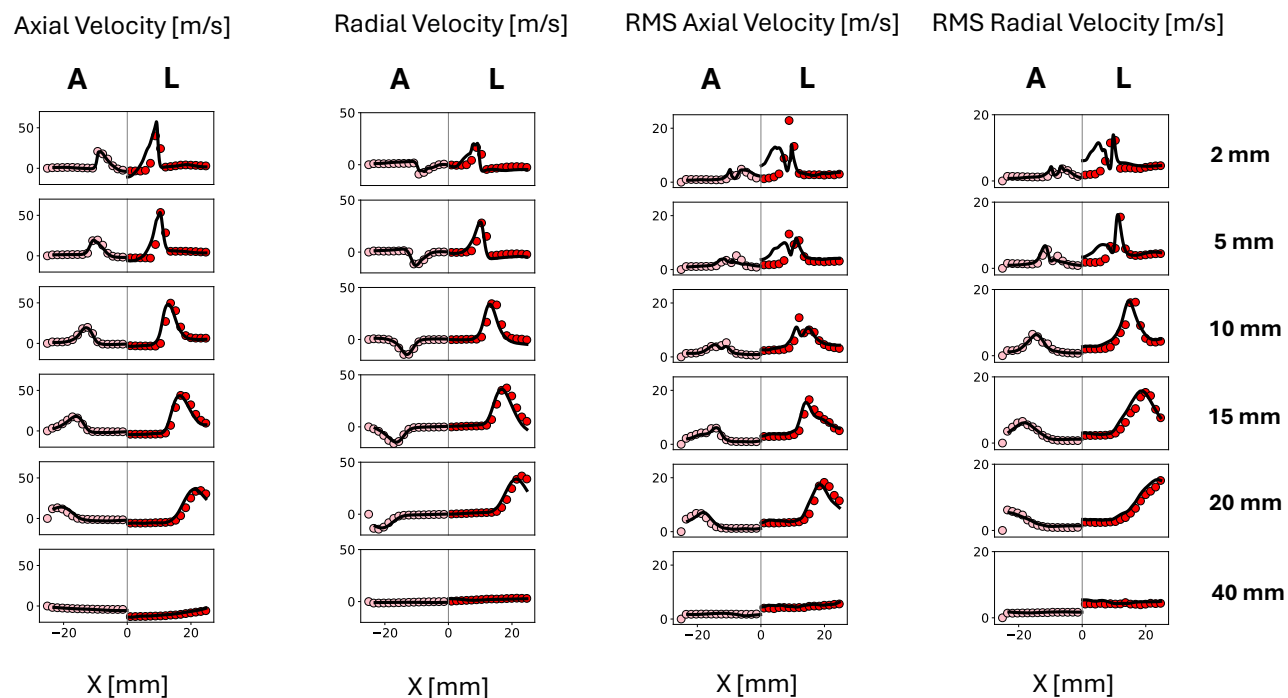


FIGURE 16: HYLON REACTIVE FLOW SIMULATION OF BOTH A (LEFT) AND L (RIGHT) CONFIGURATION (LES: —, EXP: CIRCLES)

the isothermal conditions. In addition, the model is able to capture the flame location and shape, although some discrepancies arise in the prediction of the thickness of the flame brush. As far as the non-premixed flame is concerned, results show a better agreement with the experimental data compared to the premixed case. The model is able to predict the velocity field in both the

non-reactive and reactive flow, with only some discrepancies in the prediction of the velocity fluctuations in the inner recirculation zone. The flamelet models used in these simulations are able to predict the shape of the flame and the peak location of heat release rate. Considering the prediction of the flame shape, the simulation has turned out more accurate for the anchored con-

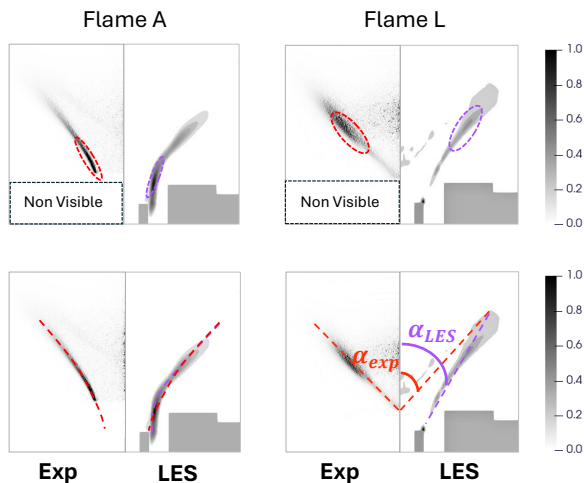


FIGURE 17: COMPARISON BETWEEN THE EXPERIMENTAL DATA (---) AND THE TIME-AVERAGED OH* MASS FRACTION (---). IN THE TWO FIGURES AT THE TOP THE ZONES WITH THE LARGEST RELEASE OF ENERGY DUE TO COMBUSTION ARE HIGHLIGHTED. THE FIGURES BELOW SHOW A COMPARISON OF THE OPENING ANGLE OF THE FLAME α BETWEEN THE EXPERIMENTAL DATA α_{exp} AND NUMERICAL RESULTS α_{LES} .

figuration than for the lifted one. Conversely, the most accurate prediction of the averaged static temperature at the exhaust was obtained for the lifted flame. The outcomes of this study comprehensively validate LES and flamelet methods, contributing to more informed selection of numerical frameworks for industrial simulation scenarios.

7. ACKNOWLEDGEMENTS

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APPENDIX A. RESOLVED TURBULENT KINETIC ENERGY

NTNU case

The contour plot of the Cèlik criterium for the NTNU test case is shown in Fig. 20. Results are reported for an x - y plane passing through the axis of the bluff-body and for three planes orthogonal to the bluff-body’s axis and located at different axial positions.

HYLON case

Figures 21 and 22 show the contour plots of the Cèlik criterium for flame A and L, respectively. Also in this case, the overall resolved turbulent kinetic energy is above 80%.

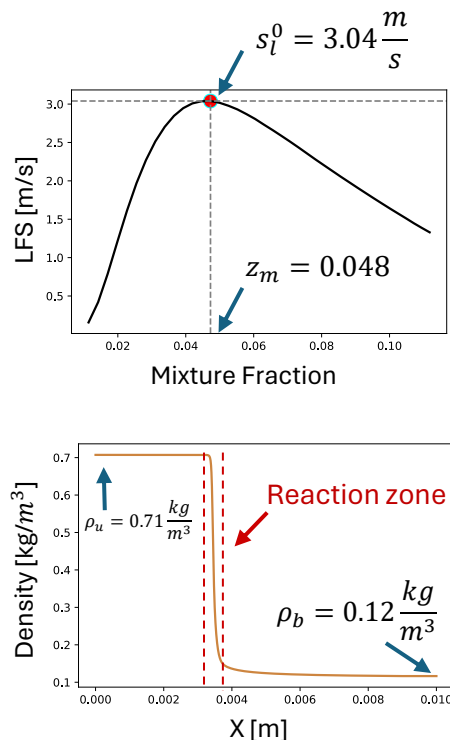


FIGURE 18: CANTERA SIMULATIONS OF THE FREELY PROPAGATING PREMIXED FLAMES FOR THE CALCULATION OF THE s_d . THE TOP FIGURE ON SHOWS THE CALCULATION OF THE MAXIMUM BURNING LAMINAR VELOCITY s_l^0 . THE FIGURE BELOW SHOWS THE CALCULATION OF THE VOLUMETRIC EXPANSION ρ_u/ρ_b OF THE GASES DUE TO THE COMBUSTION PROCESS FOR A FREELY PROPAGATING PREMIXED FLAME WITH A MIXTURE FRACTION OF Z_m .

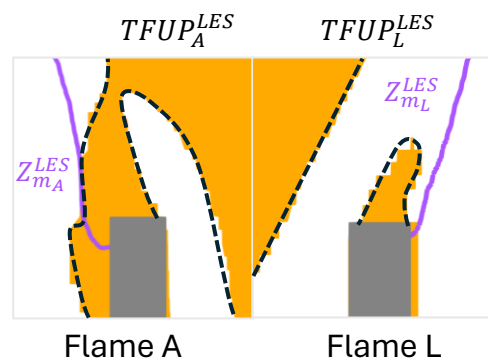


FIGURE 19: TFUP MODEL PROPOSED BY MARRAGOU ET AL [11]. THE PURPLE LINE (—) REPRESENTS THE ISOCONTOUR OF THE MIXTURE FRACTION AT WHICH THE MAXIMUM LAMINAR BURNING VELOCITY OCCURS. THE TFUP IS COLOURED IN ORANGE AND REPRESENTS THE ZONE OF THE FLOW WHERE THE MEAN AXIAL VELOCITY IS LOWER THAN THE TRIPLE FLAME SPEED s_d .

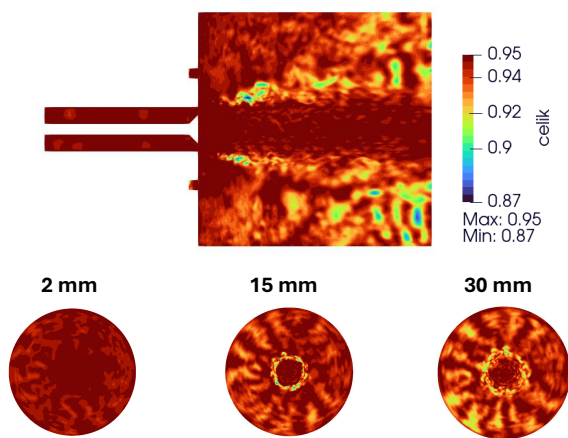


FIGURE 20: CONTOUR PLOT OF THE CELIK CRITERIUM FOR LES QUALITY IN THE REACTIVE FLOW SIMULATION FOR THE NTNU TEST CASE.

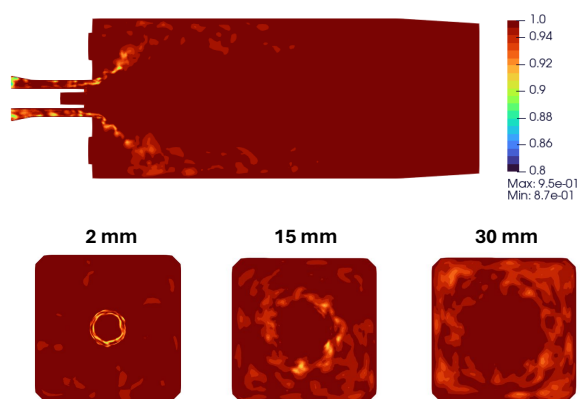


FIGURE 21: HYLON CONTOUR PLOT OF THE CELIK CRITERIUM FOR LES QUALITY IN THE REACTIVE FLOW OF THE ANCHORED FLAME.

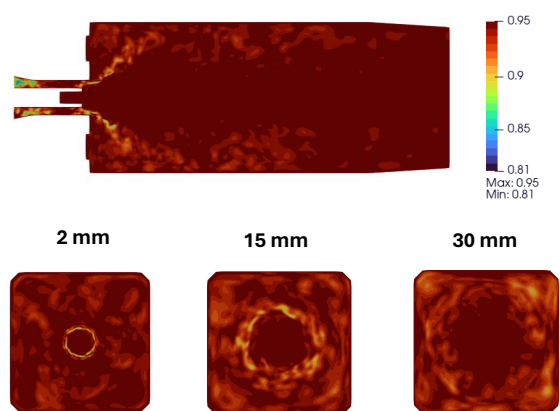


FIGURE 22: HYLON CONTOUR PLOT OF THE CELIK CRITERIUM FOR LES QUALITY IN THE REACTIVE FLOW OF THE LIFTED FLAME.

REFERENCES

- [1] Milton, BE and Keck, JC. "Laminar burning velocities in stoichiometric hydrogen and hydrogen-hydrocarbon gas mixtures." *Combustion and flame* Vol. 58 No. 1 (1984): pp. 13–22.
- [2] Bouvet, N., Halter, F., Chauveau, C. and Yoon, Y. "On the effective Lewis number formulations for lean hydrogen/hydrocarbon/air mixture." *International Journal of Hydrogen Energy* Vol. 38 (2013): pp. 5949–5960.
- [3] Sánchez, Antonio L and Williams, Forman A. "Recent advances in understanding of flammability characteristics of hydrogen." *Progress in Energy and Combustion Science* Vol. 41 (2014): pp. 1–55.
- [4] Liu, Wenjing, Sun, Lu, Li, Zhaoling, Fujii, Minoru, Geng, Yong, Dong, Liang and Fujita, Tsuyoshi. "Trends and future challenges in hydrogen production and storage research." *Environmental science and pollution research* Vol. 27 (2020): pp. 31092–31104.
- [5] Mira, Daniel, Lehmkuhl, Oriol, Both, Ambrus, Stathopoulos, Panagiotis, Tanneberger, Tom, Reichel, Thoralf G, Paschereit, Christian Oliver, Vázquez, Mariano and Houzeaux, Guillaume. "Numerical characterization of a premixed hydrogen flame under conditions close to flashback." *Flow, Turbulence and Combustion* Vol. 104 (2020): pp. 479–507.
- [6] Ganguly, R and Puri, Ishwar K. "Non premixed flame control with microjets." *Experiments in fluids* Vol. 36 (2004): pp. 635–641.
- [7] Landry-Blais, Alexandre, Sivić, Sani and Picard, Mathieu. "Micro-mixing combustion for highly recuperated gas turbines: effects of inlet temperature and fuel composition on combustion stability and NOx emissions." *Journal of Engineering for Gas Turbines and Power* Vol. 144 No. 9 (2022): p. 091014.
- [8] McAllister, Sara, Chen, Jyh-Yuan and Fernandez-Pello, A Carlos. *Fundamentals of combustion processes*. Vol. 304. Springer (2011).
- [9] Nemitallah, Medhat A, Abdelhafez, Ahmed A and Habib, Mohamed A. *Approaches for clean combustion in gas turbines*. Springer (2020).
- [10] Gao, Yupeng, Zhang, Xiaoguang, Han, Wang, Li, Jingxuan and Yang, Lijun. "Effects of swirl number and bluff body on swirling flow dynamics." *AIP Advances* Vol. 13 No. 2 (2023).
- [11] Marragou, S, Magnes, Hervé, Aniello, A, Guiberti, TF, Selle, L, Poinot, T and Schuller, T. "Modeling of H2/air flame stabilization regime above coaxial dual swirl injectors." *Combustion and Flame* Vol. 255 (2023): p. 112908.
- [12] Æsøy, E. and Dawson, James R. "TNF workshop." (2023). Accessed 2024-11-27, URL <https://tnfworkshop.org/bluff-body-hydrogen-flame-ntnu-trondheim/>.
- [13] Giusti, Andrea and Mastorakos, Epaminondas. "Turbulent combustion modelling and experiments: Recent trends and developments." *Flow, Turbulence and Combustion* Vol. 103 No. 4 (2019): pp. 847–869.
- [14] Aniello, Andrea, Laera, Davide, Marragou, Sylvain, Magnes, Hervé, Selle, Laurent, Schuller, Thierry and

- Poinsot, Thierry. "Experimental and numerical investigation of two flame stabilization regimes observed in a dual swirl H₂-air coaxial injector." *Combustion and flame* Vol. 249 (2023): p. 112595.
- [15] Ballotti, Andrea, Castellani, Simone and Andreini, Antonio. "A Dynamic Thickening Strategy for High-Fidelity Computational Fluid Dynamics Analyses of Multi-Regime Combustion." *Journal of Engineering for Gas Turbines and Power* Vol. 146 No. 12 (2024).
- [16] Kutkan, Halit, Amato, Alberto, Campa, Giovanni, Tay-Wo-Chong, Luis and Æsøy, Eirik. "LES of turbulent premixed CH₄/H₂/air flames with stretch and heat loss for flame characteristics and dynamics." *Turbo Expo: Power for Land, Sea, and Air*, Vol. 86007: p. V03BT04A021. 2022. American Society of Mechanical Engineers.
- [17] Kutkan, Halit, Amato, Alberto, Campa, Giovanni, Ghirardo, Giulio, Tay Wo Chong, Luis and Æsøy, Eirik. "Modeling of turbulent premixed CH₄/H₂/air flames including the influence of stretch and heat losses." *Journal of Engineering for Gas Turbines and Power* Vol. 144 No. 1 (2022): p. 011020.
- [18] Amerighi, Matteo, Senatori, Giada, Yahou, Tarik, Schuller, Thierry, Dawson, James R and Andreini, Antonio. "Complete Dynamics From Ignition to Stabilization of a Lean Hydrogen Flame With Thickened Flame Model." *Journal of Engineering for Gas Turbines and Power* Vol. 147 No. 4 (2025).
- [19] Yahou, T, Detomaso, N, Selle, Laurent, Poinsot, Thierry, Dawson, JR, Schuller, Thierry and Laera, D. "The role of preferential diffusion on the ignition dynamics of lean premixed hydrogen flames." *Proceedings of the Combustion Institute* Vol. 40 No. 1-4 (2024): p. 105612.
- [20] Yahou, Tarik, Dawson, James R and Schuller, Thierry. "Impact of chamber back pressure on the ignition dynamics of hydrogen enriched premixed flames." *Proceedings of the Combustion Institute* Vol. 39 No. 4 (2023): pp. 4641–4650.
- [21] Æsøy, Eirik, Aguilar, José G, Bothien, Mirko R, Worth, Nicholas A and Dawson, James R. "Acoustic-convective interference in transfer functions of methane/hydrogen and pure hydrogen flames." *Journal of Engineering for Gas Turbines and Power* Vol. 143 No. 12 (2021): p. 121017.
- [22] Æsøy, Eirik, Nygård, Håkon T, Worth, Nicholas A and Dawson, James R. "Tailoring the gain and phase of the flame transfer function through targeted convective-acoustic interference." *Combustion and Flame* Vol. 236 (2022): p. 111813.
- [23] Æsøy, Eirik, Jankee, Girish K, Yadala, Srikar, Worth, Nicholas A and Dawson, James R. "Suppression of self-excited thermoacoustic instabilities by convective-acoustic interference." *Proceedings of the Combustion Institute* Vol. 39 No. 4 (2023): pp. 4611–4620.
- [24] ANSYS. "ANSYS FLUENT User's Guide, Version 12.0." Accessed 2024-11-27, URL <https://www.afs.enea.it/project/neptunius/docs/fluent/html/th/node156.htm>.
- [25] Zimont, Vladimir, Polifke, Wolfgang, Bettelini, Marco and Weisenstein, Wolfgang. *An efficient computational model for premixed turbulent combustion at high Reynolds numbers based on a turbulent flame speed closure*. Vol. 78699. American Society of Mechanical Engineers (1997).
- [26] Smith, Gregory P., Golden, David M., Frenklach, Michael, Moriarty, Nigel W., Eiteneer, Boris, Goldenberg, Mikhail, Bowman, C. Thomas, Hanson, Ronald K., Song, Soonho, Jr., William C. Gardiner, Lissianski, Vitali V. and Qin, Zhiwei. "Current and Future Releases of GRI-Mech."
- [27] Nori, Venkata and Seitzman, Jerry. "Evaluation of chemiluminescence as a combustion diagnostic under varying operating conditions." *46th AIAA Aerospace Sciences Meeting and Exhibit*: p. 953. 2008.
- [28] Tyacke, James C and Tucker, Paul G. "Future use of large eddy simulation in aero-engines." *Journal of Turbomachinery* Vol. 137 No. 8 (2015): p. 081005.
- [29] Celik, IB, Cehreli, ZN and Yavuz, I. "Index of resolution quality for large eddy simulations." *Journal of Turbomachinery* (2005).
- [30] Kai, Reo, Tokuoka, Taiki, Nagao, Jun, Pillai, Abhishek Lakshman and Kurose, Ryoichi. "LES flamelet modeling of hydrogen combustion considering preferential diffusion effect." *International Journal of Hydrogen Energy* Vol. 48 No. 29 (2023): pp. 11086–11101.
- [31] Klarmann, Noah, Sattelmayer, Thomas, Geng, Weiqun and Magni, Fulvio. "Flamelet generated manifolds for partially premixed, highly stretched and non-adiabatic combustion in gas turbines." *54th AIAA Aerospace Sciences Meeting*: p. 2120. 2016.
- [32] Knudsen, E and Pitsch, H. "Capabilities and limitations of multi-regime flamelet combustion models." *Combustion and Flame* Vol. 159 No. 1 (2012): pp. 242–264.
- [33] Luo, Yujuan, Steinhausen, Matthias, Kaddar, Driss, Hasse, Christian and Ferraro, Federica. "Assessment of flamelet manifolds for turbulent flame-wall interactions in large-eddy simulations." *Combustion and Flame* Vol. 255 (2023): p. 112923.
- [34] Goodwin, David G., Moffat, Harry K., Schoegl, Ingmar, Speth, Raymond L. and Weber, Bryan W. "Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes." <https://www.cantera.org> (2023). DOI 10.5281/zenodo.8137090. Version 3.0.0.