High-fidelity investigation of FGM and TFM approach on a lean hydrogen flame

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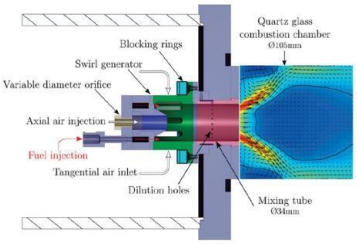
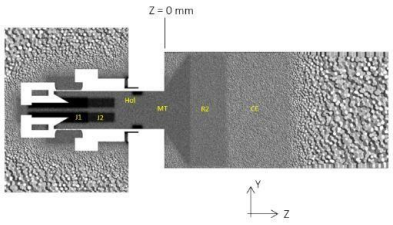
Abstract
Climate change due to carbon emissions is one of the aspects that must be kept under control nowadays. In this fashion, the employment of hydrogen as fuel provides a fundamental solution for both power generation and transportation since lean premixed combustions allow to reset the carbon emissions and limit the NOx ones. The present work aims to study through two different numerical approaches a technically premixed hydrogen flame experimentally investigated at the Berlin Institute of Technology (TUB). The comparison with the experimental data shows the treatment employed drastically influences the obtained outcomes.

Introduction
Hydrogen combustion systems are nowadays studied and developed by many companies and universities since their employment as fuel is considered a valid alternative to reach net-zero CO_2 emission by 2050 [1]. Specifically, lean premixed or technically premixed configurations [2-3] are of great interest because they allow to control the temperature in the primary zone to limit the NOx emissions.
However, lean conditions can drastically increase the flashback and lean blow-off risk. Moreover, hydrogen is characterized by a higher mass diffusivity with respect to the thermal one which can impact both its dynamics and stabilization mechanism since it modifies the flame response to the stretch. This effect is referred in the literature as preferential diffusion [4].
From a numerical point of view, proper modeling is not straightforward since different aspects must be considered.
A strategy can be found in the tabulated chemistry approach in which through a detailed reaction mechanism a look-up table is generated and queried at runtime using the selected control variables and their respective variances. In this way, the reaction occurs as a single-step chemistry, and all the information about the mixing is described with a single variable (e.g., mixture fraction). Without modifications to the original formulation as presented in [5], the preferential diffusion effects are not included.
A second strategy instead can be found in the species transport approach which directly resolves a transport equation for each species involved in the employed reaction mechanism. In this way, each species is characterized by its mass and

thermal diffusivity allowing from a theoretical point of view to include the preferential diffusion effects. Moreover, it is also possible to describe the reactivity of a mixture with different reaction time scales according to the selected reaction mechanism.

The present work aims to assess the results obtained with the aforementioned strategies on a lean, swirl-stabilized, technically premixed hydrogen flame. In the first part of the paper, an explanation of the models employed will be presented. Then, a brief description of the investigated test case will be provided with the numerical strategy used. In the last part of the paper, a detailed comparison of the results obtained and a comparison with the available experimental data will be shown.





Sizing	
Global	5 mm
CC	1 mm
R2	600 µm
MT	450 µm
J2	200 µm
J1	100 µm
Hol	100 µm

Figure 1. (Left) Experimental test case [3]. (Center-Right) Numerical grid with relative sizing.

Experimental test rig

The rig under investigation is the burner developed during the AHEAD project provided by the Berlin Institute of Technology (TUB) [3] (Fig.1). The quartz combustion chamber has an internal diameter of 104 mm, and it is feds through a mixing tube in which air and fuel mix together reaching technically premixed conditions. The fuel was injected through sixteen holes placed at the bottom of the mixing tube while the air is provided in two different ways. The first one is a pure axial injection characterized by a high momentum aiming to prevent the flashback risk while the second one is a modular swirler which can be adjusted by adding or removing blocking rings. In the present work, the long mixing tube (60 mm) configuration with the maximum axial momentum is analyzed (d_{ax} = 8.8mm and two blocking rings with 7 mm blockage height). The chamber operates under atmospheric conditions with a nominal equivalence ratio of ϕ = 0.6. The air was preheated at 623.15 K and a constant mass flow rate of 130 kg/h feds the plenum while the fuel was provided at 352.15 K. Detailed measurements are available for both non-reactive (PIV) and reactive (PIV and OH-PLIF) conditions. The readers interested in more detailed information about the experimental facilities are referred to [3].

Numerical setup

From a numerical point of view, the commercial pressure-based code ANSYS Fluent 2019R3 is used for all the simulations in the unsteady high-fidelity LES framework. The domain is discretized starting from the air plenum up to the outlet including the swirler, the fuel plenum and the dilution holes located in the middle of the mixing tube. A polyhedral mesh was generated counting roughly 29M elements with ad-hoc refinements at the exit of the axial jet and inside the combustion chamber (Fig.1). For all the simulations, a constant mass flow rate of air and fuel is imposed at the inlet patches, whereas constant pressure is prescribed at the outlet. All the other surfaces are representative of solid walls, so the no-slip conditions are imposed with an adiabatic condition since no information is available for the thermal boundary.
The effect of unresolved eddies is modeled using the Dynamic Smogorinsky-Lilly formulation which dynamically evaluates the Smagorinsky constant. For the tabulated chemistry simulation (named FR in the following), the Flamelet Generated Manifold (FGM) [4] with two control variables (mixture fraction Z and progress variable c) is used to account for the turbulence-chemistry interaction. The un-normalized progress variable is defined as $Y_c = Y_{H_2O} - Y_{H_2}$as deeply explained in [6]. For the laminar look-up table generation, several premixed freely propagating flames were calculated using the detailed ELTE reaction mechanism.
For the species transport simulation instead, the Thickened Flame Model (TFM)[7] is used in which the thermal thickness was described with 5 points. The thickening is dynamically applied only in a narrow band of the flame front thanks to a sensor factor and the sub-scale wrinkling effects were retrieved with the Colin [7] efficiency function. The Boivin mechanism [8] (9S with 12R) is used to describe the reactivity and a mixture-average approach is adopted to evaluate the mass diffusivity according to the kinematic theory. A constant time step of $1.0 \times 10^{-06}s$ is used for both simulations ensuring a convective Courant number below 10 in the zones of interest.

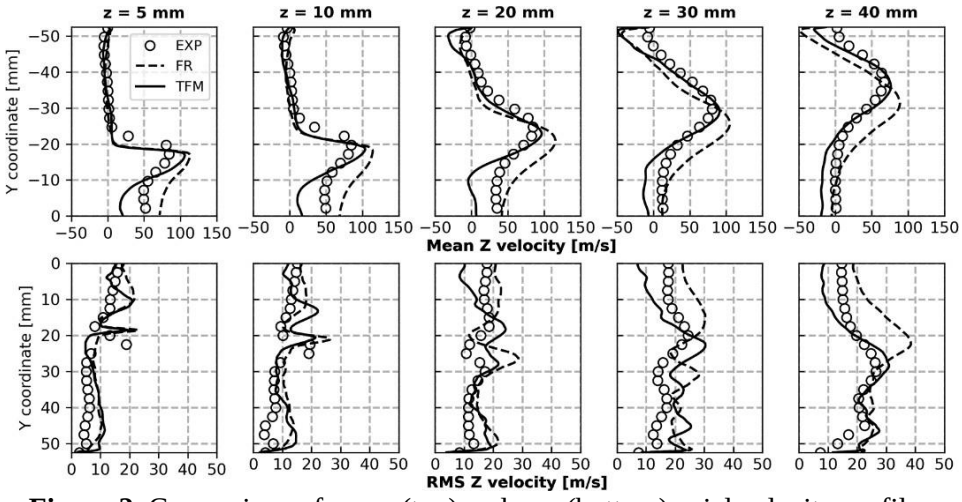


Figure 2. Comparison of mean (top) and rms (bottom) axial velocity profiles.

Results

In this section, a deep analysis of reactive results obtained with the FR and TFM models will be presented. The validation of the non-reactive flow field with a mesh sensitivity is not reported here for the sake of brevity, the reader interested in more details about that is referred to [6]. A comparison in terms of mean and root mean square of axial velocity on five heights inside the combustion chamber is reported in Fig.2. A very good agreement with the experimental data can be pointed out for both simulations at all stages.

It is important to highlight a better prediction of the flow field of the TFM simulation especially at high stages in which the correct opening of the swirling jets is well reconstructed. This is probably caused by the lower velocity at the exit of the mixing tube with respect to the FR case which increases the actual swirl number. Thanks to the local refinements generated in the reaction zone, also the velocity fluctuations in the axial direction are well reconstructed by the simulations even if the FR case slightly overestimates the experimental one.

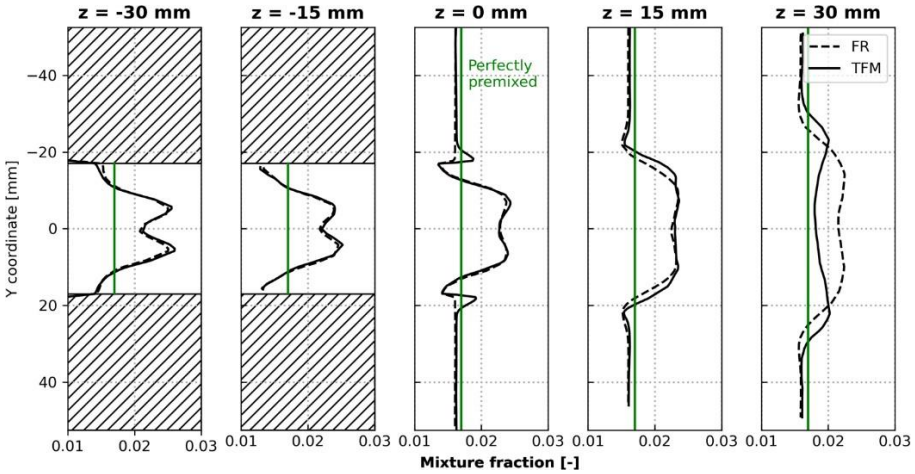


Figure 3. Mean mixture fraction profiles at different heights.

Moving to the mixing process, the mean mixture fraction distribution over five stages across the burner is reported in Fig.3. It is important to highlight that no differences appear between the models inside the mixing tube even if the FR equations are written with the Unity Lewis assumption. This confirms that the preferential diffusion effects affect only the zones in which the reactions take place, as can be observed at the exit of the mixing tube (z = 0 mm, y ≈ ± 20 mm) in which the TFM retrieves a peak of mixture fraction, as will be better explained later. In the plots are also superimposed a green line at the nominal value ($\phi = 0.6$) at which the rig operates. Even in the long mixing tube configuration, only at z > 30 mm the nominal composition is retrieved, showing the technically premixed condition at which the burner operates.

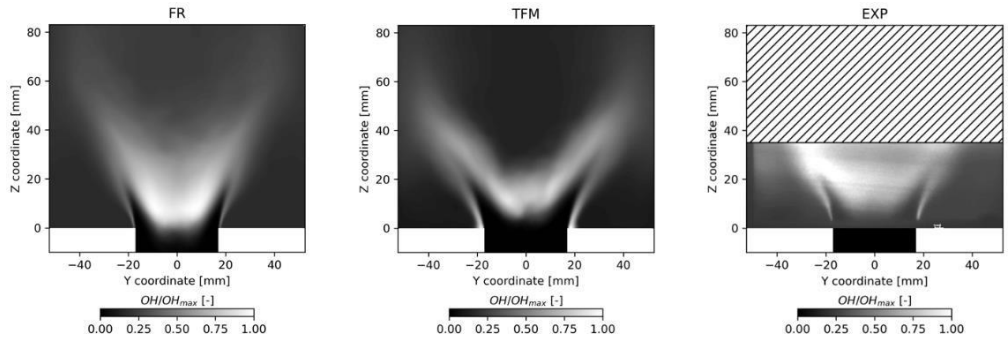


Figure 4. Normalized OH mass fraction distribution.

To validate the flame shape, a comparison in terms of normalized OH mass fraction is performed in Fig.4 in which the numerical maps are compared with the normalized OH-PLIF image (cropped above 35 mm to highlight the stabilization zone). In the FR solution, the flame stabilizes around the exit of the mixing tube due to the higher reactivity of the numerical approach employed. However, from the TFM simulation, the correct flame position and shape are retrieved with respect to what was observed experimentally. In both cases, the flame is attached to the mixing tube exit corner which is probably related to the adiabatic conditions imposed in such walls, as pointed out in [9]. It is also important to highlight the high reactivity observed in such zones from the TFM simulations due to the preferential diffusion effects which locally create a richer mixture (with respect to the FR value, see again Fig.3).
To better investigate this phenomenon, the local temperature probability density functions over the mixture fraction are reported in Fig.5 for the two simulations. A black isoline of the equilibrium temperature computed from its relative reaction mechanism is superimposed in the plots. Histograms of both quantities are also reported dividing the region between the Inner (ISL) and Outer (OSL) Shear Layer. The first observation that can be drawn by analyzing the histogram is the clear presence of a second peak of reactions that occur on the OSL in the TFM results.

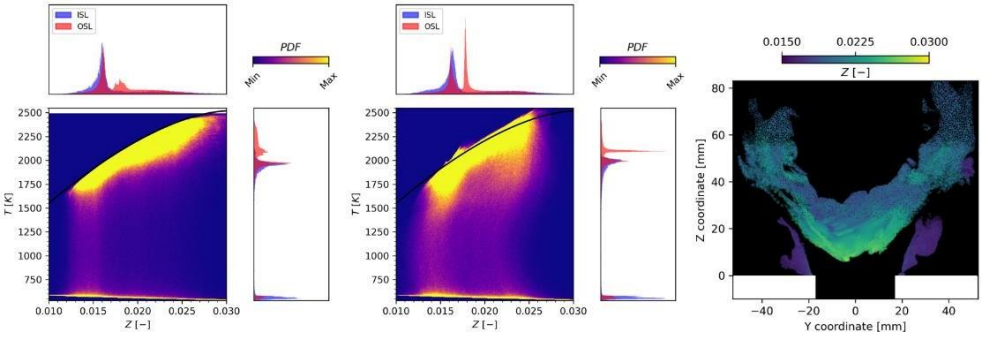


Figure 5. (Left-Center) 2D PDF of temperature and mixture fraction for FR and TFM respectively. (Right) Conditioned scatter plot of mixture fraction for TFM.

Moreover, it is possible to point out how the maximum temperature is always below the equilibrium one in the FR simulation according to the PDF. Instead, in the TFM case, some zones of the domain reach a temperature higher than the one at the equilibrium. This phenomenon is referred in the literature as super-equilibrium and occurs due to the preferential diffusion effects (which act on the high-strain regions [4]). To localize such points, in the last plot of Fig.5 a conditioned scatter plot colored by the local mixture fraction is reported (points with $T > T_{eq}$). In this way is possible to see that the first region (Z ≈0.017) is located on the outer shear layer (where the strain is higher) as previously mentioned while the second one, at a higher mixture fraction (Z>0.02), is located on the stabilization zones in the ISL.

Conclusion

In the present work, a technically premix, swirl-stabilized hydrogen flame is numerically investigated through high-fidelity Large Eddy Simulations. Two turbulence combustion models based on different approaches are tested and the results are compared with the available experimental data provided by the TUB. The TFM model better predicts the flame shape thanks to the inclusion of preferential diffusion effects which locally modify the fuel distribution and flame dynamics.

Nomenclature

c	Progress variable
T	Temperature
Z	Mixture fraction
ϕ	Equivalence ratio

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