Numerical Modelling of Swirl Stabilised Lean-Premixed H_2-CH_4 Flames with the Artificially Thickened Flame Model

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Abstract

In this work, high-fidelity simulations of perfectly premixed swirl stabilized flames have been performed varying the H2 content in the fuel from 0 to 100% to investigate the effect of the hydrogen addition on a natural gas fired combustor. The artificially thickened flame model (ATFM) has been used to treat the turbulent chemistry interaction. The numerical results have been compared with the detailed experimental data performed at Cardiff University's Gas Turbine Research Centre showing a very good prediction accuracy.

Introduction

Hydrogen integration into the gas turbine combustion systems requires significant changes in the combustor architecture. Nevertheless, dealing with hydrogen, one of the most attractive solutions is still the lean premixed technology, representing nowadays the state of the art for low carbon fuel combustion in land-based gas turbines. The enabling of Dry-Low NOx (DLN) technology to high H2 content allows the exploitation of part of the industry's know-how acquired over years for Natural Gas (NG) combustion. Moreover, starting the redesign process from configurations already capable to manage the NG combustion, would help to preserve a certain degree of retrofitting and fuel flexibility. In the transitional phase toward using carbon-free fuels, the new combustion systems need to ensure fuel flexibility overcoming the discontinuous hydrogen supply.

The lean premixed burner design could face several difficulties related to the different thermodynamic and chemical properties of H2 with respect to conventional fuels. Due to the higher adiabatic flame temperature of H2 with respect to CH4, H2-fueled systems must be operated in leaner conditions to contain NOx emissions. Moreover, the high H2 reactivity rises the flashback risk altering the stability margin of the combustor and worsening its operability under low loads.

All these arguments rise the need to experimentally investigate the effect of H2 addition in lean-premixed conditions, likewise, validating the numerical model prediction capacity.

The combustion modelling of high hydrogen-containing mixtures must be able to account for the differential diffusion to correctly characterize the flame propagation characteristics. The species transport models are intrinsically capable to account for all these aspects on the solved flame front. In this work, the Artificially Thickened Flame Model (ATFM) [1] has been adopted to model the turbulence chemistry interaction.
The CH4-H2 lean premixed flames have been heavily studied in the literature with both experimental and numerical work. Agostinelli et al. [2] have recently investigated the PRECCINSTA burner operated up to 50%vol of H2 with CH4 under pressure, highlighting how the computational cost rises sharply with the pressure increase with H2. Nevertheless, the prediction capability of the ATFM in these conditions is excellent as it also shows an accurate reconstruction of the thermoacoustic behaviour. To the authors' knowledge, no single study in the literature considers H2 contents from 0% up to 100% on lean premixed swirl stabilized flames. This work aims to investigate the effect of hydrogen addition from 0% to 100% on the flame morphology experimentally and numerically. Moreover, the measured OH* chemiluminescence allows the validation of the ATFM prediction capacity when preferential diffusion effects are expected to be essential for flame propagation.

Experimental Facility

The test case studied in this work has been investigated during the experimental campaign conducted in the GTRC laboratory at Cardiff university research centre. The facility (described in detail in [3]) consists of a high-pressure rig with optical accesses. The air supply line includes an electric heater that allows the mixture to reach a temperature of up to 573 K with a flow capacity of 0.25 kg/s. The facility is equipped with a radial-tangential swirler (having geometric swirl number 0.8) based on industrial lean premixed design. In the context of this study, the burner has been operated in fully premixed conditions and the whole rig is at atmospheric pressure.
The high-speed OH*chemiluminescence image capture system utilizes a combination of a high-speed camera, relay lens, high-speed image intensifier, UV lens (RicohFL-GC7838-VGUV, f/8) with a 310nm narrow bandpass filter.

Computational domain and numerical setup

The test case just introduced has been numerically investigated with high-fidelity LES simulations. The spatially filtered Navier Stokes equations have been solved with the pressure-based solver ANSYS Fluent 2022R2. The turbulent combustion has been modelled with the ATFM with constant thickening since all the investigated cases are perfectly premixed. Nevertheless, the thickening is only applied on the flame front using a dynamic thickening factor. Sub-scale wrinkling effects have been taken into account through the efficiency function formulation proposed by Colin et al. [1]. Most of the efficiency function formulations require the estimation of the dilatation-free velocity fluctuation at the test filter. Colin et al. [1], have proposed a

formulation that requires the third-order derivative of the filtered velocity, a non-trivial task on an unstructured mesh. Instead, the approach proposed by Durand et al. [4] is adopted here.
A 26 species and 119 reactions skeletal mechanism derived from the UCSD mechanism is employed; the chemistry set was retrieved leveraging the commercial code CHEMKIN-Pro and a detailed description of the reduction procedure can be found in the work of Meloni et al [5]. The chemical source terms are computed using a stiff chemistry solver, that allows the decoupling of the chemical timestep with the simulation timestep.

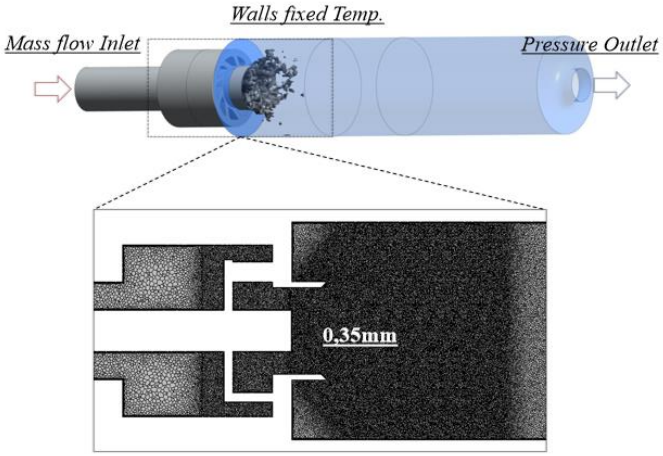

Figure 1 Schematic visualization of the computational domain, and mesh with the refinement zone

The computational domain is shown in Figure 1. All the walls are treated with a wall function approach and a fixed temperature is imposed on the different quartz tube regions according to the measurements.
The mesh for all the investigated conditions counts 16 million polyhedral elements. The refinement zone is shown in Figure 1, and includes the swirler and all the expected flame regions with an average size of the elements of 0.35mm. Three prismatic layers have been placed on the walls in order to improve the discretization of the boundary layer. Some information about the test points investigated are reported in Table 1.

Table 1 Summary of test points investigated

	0H2	**60H2L**	**100H2L**
%H2 by vol. [-]	0%	60%	100%
Φ [-]	0.6	0.465	0.265
$\boldsymbol{F_{max}}$	5.4	5.2	3.3
LFS	0.38	0.36	0.2
$\boldsymbol{T_{ad}[K]}$	1822	1608	1277

u_{bulk}[m/s]	21.1	26.5	41.4

Results

The OH* radical is solved to be directly compared with the experimental OH* chemiluminescence signal. In Figure 2 the time-average Line Of Sight (LOS) of the Y^*_{OH} has been compared with the experimental OH* chemiluminescence for all the investigated test points. In all the conditions the model prediction shows an overall good agreement with the experimental measurements. Experimentally, the flame is V-shaped and its length is very sensitive to the change in the inlet mass flow and %H2. The flame morphology is well reconstructed by the model that successfully captures the flame extinction on the external shear layer. Moreover, also the flame length variation with H2 addition is well predicted. The simulations underestimate slightly the flame length decreasing the H2 content. This discrepancy may be ascribable to the near-wall flame heat loss characterization since, for the 0% H2 case, the flame interacts with the wall making the uniform wall temperature boundary a less realistic assumption. It can be easily seen that the increase in the H2 content of the mixture finally results in a more compact flame. This suggests that the turbulent flame speed increases with the increase in the H2 content allowing a higher fuel consumption rate.

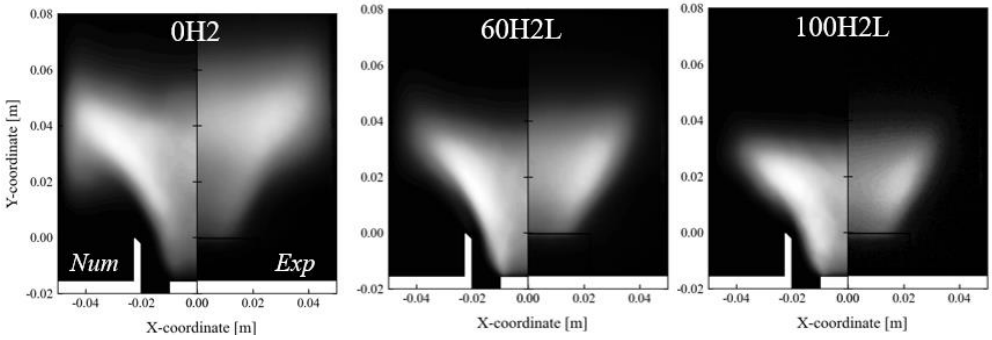

Figure 2 Comparison between the numerical time-averaged OH* LOS (left) and the experimental time-averaged OH* signal (right) for all the test points (Table 1).

This global increase in the flame reactivity moving toward higher H2 content is not explainable by the unstretched LFS of the mixture shown in Table 1. Indeed, increasing the H2 content, the LFS decreases due to the lower equivalence ratio of the mixture, but the overall turbulent flame speed S_T is found to increase leading to a shorter flame even considering the higher bulk velocity.

The dashed line in Figure represents the heat released (HR) from the reference 1D unstretched laminar flame. The scatterplot shows that the turbulent solution overestimate heavily the unstretched 1D HR increasing the H2 content. Such higher HR levels are explainable including the effect of the strain in the laminar flamelet. With this purpose, a series of laminar flamelet solutions have been reported in Figure increasing the strain rate level for each %H2 (continuous lines). The effect of the

strain combined with the H2 differential diffusion makes the unstretched solution to be not representative of the strained tri-dimensional flame front. For this reason, the flame reactivity is found to deviate from the unstretched estimation as much as the H2 content increases, thus contributing to explain the flame shortening with the H2 increase. The colour of the scatterplot in Figure represents the local level of enthalpy loss with respect to the adiabatic unburnt conditions and is evaluated as:

$$H_{rel} = \left(h_s + \sum_{k=1}^{N} Y_k \, \Delta h_{f,k}^0\right) - \left(h_s + \sum_{k=1}^{N} Y_k \, \Delta h_{f,k}^0\right)_{unburnt} \quad \textbf{Equation 1}$$

In which h_s is the sensible enthalpy, and $\Delta h_{f,k}^0$ is the formation enthalpy of the species k. Another contribution to the flame shortening is the decreasing level of H_{rel} (Figure) at which the flame is subjected, which is mainly due to the decrease of the flame temperature with the increase of the H2 content.

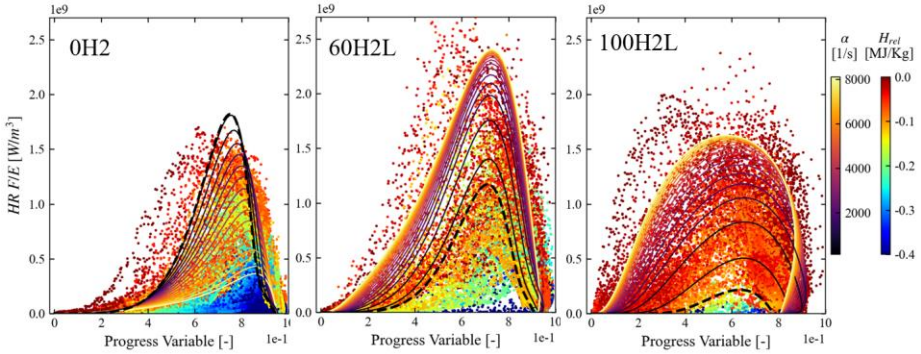

Figure 3. Scatter plot showing scaled HR respect to the normalised PV ($Y_{PV} = -Y_{H2} + Y_{H2O} + Y_{CO2} + Y_{CO}$) sampled from an instantaneous solution on the xy-plane. Colours represent the local level of H_{rel}. (Continuous lines) HR of laminar counterflow flamelet increasing α; (Dashed lines) laminar unstretched flamelet solution.

Nomenclature

F_{max}	Maximum Thickening Factor [-]
H_{rel}	Relative sensible and chemical enthalpy [MJ/kg]
Y	Species Mass Fraction [-]
S_T	Turbulent flame speed [m/s]
T_{ad}	Adiabatic burnt temperature [K]
u_{bulk}	Swirler exit bulk velocity [m/s]
α	Strain Rate [1/s]
Φ	Equivalence Ratio [-]

Acronyms

ATFM	*Artificially Thickened Flame Model*
DLN	*Dry-Low NOx*
HR	*Heat Released*
LES	*Large Eddy Simulation*
LFS	*Laminar Flame Speed [m/s]*

LOS Line Of Sight

Conclusion

A perfectly premixed swirled stabilized flame has been investigated both experimentally and numerically considering an increasing level of H2 in the H2-CH4 fuel mixture (from 0% to 100%). The accordance between the experimental OH* measurements and the numerical results proves the effectiveness of the ATFM to be predictive in the whole range of conditions.

Contrary to what may be expected, the measured and predicted flame extensions are against the mixture laminar flame speed trend. Thus, increasing the H2 content the mass flow, the flame gets shorter despite the mixture LFS estimation decreases. The comparison between the heat released of the numerical simulation with some laminar flamelet shows that the heat loss and presence of stretch on a flame front having Le<1 are two contributions that lead the reactivity to heavily differs from the unstretched adiabatic laminar condition.

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